

CHEMISTRY

# GOESSMANN GAZETTE

## UMass, Metawampe, and Chemistry

A departmental tradition woven  
into local history.

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UMassAmherst

College of Natural Sciences  
Chemistry





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Dear Alumni and Friends of UMass Chemistry,

A lot happened in the life of the Chemistry Department last year. One particularly exciting moment was learning that Prof. Lila Gierasch was elected to the National Academy of Sciences (NAS). Lila is one of only a handful of UMass Amherst faculty ever elected to this prestigious academy, and right now she is the only active UMass Amherst faculty who is a member of the NAS.



We also celebrated the long-anticipated move of several faculty and their research labs into the new Physical Science Building (PSB), which occurred right before the beginning of the Fall 2018 semester, although the 'official' opening did not happen until April 2019. That's when Governor Charlie Baker, UMass President Marty Meehan, Chancellor Kumble Subbaswamy, and many other dignitaries joined us for a well-attended ribbon-cutting ceremony. As we have written about in many recent Gazettes, PSB is an amazing state-of-the-art research space for some of the synthesis-oriented chemists in our department.

This brand-new research space helped us successfully recruit two new faculty members. James Walsh will join us in the Fall of 2019. He will teach courses in inorganic and materials chemistry while starting an exciting research program in the high-pressure synthesis of novel solid-state materials with new mechanical and magnetic properties. Joining James in PSB will be Joseph DuChene, who will teach analytical chemistry and run a research program developing new methods to understand how catalysts can utilize light selectively for desired chemical reactions. Joe will arrive in January 2020.

Sadly, we said good-bye to a long-time member of the Chemistry community, Prof. Louis Carpino, who passed away on January 4, 2019. Louis was a member of our Department for almost 65 years! He was famous for inventing the widely used t-Boc and F-moc protecting groups that revolutionized peptide synthesis. Not only did he have an incredible impact in the world of organic chemistry, he left a legacy of having trained numerous students and postdoctoral researchers.

Two other people who have had a marvelous impact on the life of our Department over the years are Prof. Michael Maroney and Ms. J. M. Stowe, who both recently retired. You can read more about both of their amazing careers in this issue of the Gazette. We are incredibly grateful to Mike and jms for their dedication to UMass Chemistry.

Starting this Fall, Prof. Ricardo Metz will be our next Department Head. He's a physical chemist who studies transition metal catalysis and has been Associate Head for several years. Our Department will be in very capable hands! It has been my pleasure to serve the Chemistry Department for the last three years. I have particularly enjoyed interacting with our incredible alumni and students who have made and continue to make UMass Chemistry an amazing place.

Finally, we continue to be grateful to all of you who have been tremendously dedicated to our Department over the years. Your generosity is inspiring. Your support helps us continue to train the next generation of chemists while at the same time pushing the boundaries of chemical knowledge.

Sincerely,

Richard Vachet, Head of Chemistry



# UMass Metawampe Hike

by Dave Adams

On Sunday, November 4, 2018, over 50 hikers, beginning in Leverett, scaled Mount Toby along some of the most biodiverse trails in Massachusetts, trekked down the other side into Sunderland, and enjoyed a well-deserved, all-you-can-eat, chicken pot pie dinner at the Sunderland First Congregational Church. Among the hikers were current and retired faculty, undergraduate and graduate students, alumni, and staff of the UMass Amherst Chemistry Department. This—incredibly—marked the 111<sup>th</sup> annual Metawampe Hike. How did this tradition begin? Where did the name originate? And how did UMass—and the Chemistry department—become involved?

The tale begins on April 10, 1674 when a local Nonotuck (sometimes called Norwottok) Chief named Metawampe sold a tract of land known as “Hunting Hills” (present day Montague) to a group of Hadley settlers represented by John Pynchon of Springfield. The land lay just north of Mt. Toby. On the same day they also purchased land that included Mt. Toby from a *sunksqua* (woman leader) named Mishalisk. The Nonotucks called Mt. Toby *Kunckquachu*, meaning “very high mountain.” In 1849, Amherst College President Edward Hitchcock proposed changing the name from Mt. Toby, which had been named in recognition of the Captian Elnathan Toby for being the first settler to climb the mountain, to Mt. Metawampe in honor of the Chief. Although the name of Mt. Toby was never officially changed, the mountain was known informally by locals as Mount Metawampe for many decades.

Thus, when faculty and staff of the Massachusetts Agricultural College (MAC) formed a hiking/outing club in 1907, they called it the Metawampe Outing Club since it was on and over this mountain they regularly hiked. The Club had a constitution and officers including president, treasurer, and trekmaster. The Metawampe Club organized and conducted its first “Metawampe Hike” in 1908. This became an annual trek over and around Mt. Toby and other local mountains on different trails, usually held in the fall after the semester ended. On November 27, 1916, MAC bought 755 acres of forested land (721 in Sunderland and 34 in Leverett) that included Mount Toby for \$30,000. The MAC forestry department proposed to use the tract, currently known as the Mount Toby State Demonstration Forest, in support of their academic programs. None of this land was part of the original tract deeded by Metawampe in 1674, but much of it was part of the tract Mishalisk sold that same year. After the college purchased Mt. Toby, the outing club standardized the route of the Metawampe Hike so that it always went over Mt. Toby from Leverett to Sunderland. The hikers spent so much time on the mountain that the Metawampe Club decided to build a log cabin in a hemlock and chestnut grove on the slopes of Roaring Hill in early 1921.

A committee consisting of Agricultural Experiment Station Director **Henry Haskell**, Professors **Frank A. Waugh** (the Frank A. Waugh Arboretum covers much of the UMass Amherst campus), **Lawrence Grose**, **Curry S. Hicks** (UMass Athletic Director), and **Arthur K. Harrison** (Instructor of Landscape Architecture), and college photographer **Bob Coffin** (known for his bird and nature photography), chose the spot for the cabin. The 12' by 15' cabin, built with chestnut logs then recently felled by the forestry department in their efforts to clear the forest of Asian blight diseased chestnut trees, had a 4' fireplace and 2 bunks. Chemistry Professor **Charles A. Peters**, **MAC Class of 1897**, the person for whom Peters Auditorium in Goessmann Laboratory is named, was responsible for “chinking” (the process of applying the flexible sealant) between the chestnut logs as part of the



Dave Adams (center) with his daughter Eileen Adams '88 & '90 (right), and granddaughter Brooke (left)



Group photo of 2018 hikers



Metawampe Club cabin





Building the Metawampe Club cabin 1921



View of Mt. Sugarloaf from the Mt Toby Fire Tower



Mount Toby Fire Tower

original building crew, and later on, replacing broken windows and old floor boards as needed. The cabin sheltered hikers regularly for the next sixty years, and served as a resting point for the annual Metawampe Hike as well as overnight accommodations at other times. Over the years the Club position of Keeper of the Cabin was instituted and involved cabin maintenance and refreshment preparation. Chemistry Department Keepers included Professor **Everett Reed, '77 PhD** and Professor **Earl McWhorter**. Beginning in the early 1960s, the structure fell into increasing disrepair. When the roof collapsed in the 1990s, deterioration escalated, and alas, only remnants remain visible today.

Back in the early 1900's, the Metawampe Club consisted of men only, so the MAC women hikers formed their own group and built a cabin on Ox Hill, which is located on the other side of Roaring Brook from the men's cabin. Unfortunately, the Great Hurricane of September 21, 1938, which caused unprecedented damage as it traveled up the Connecticut River, destroyed the women's cabin, and it was not rebuilt.

As MAC became Massachusetts State College (MSC) in 1931 and MSC became the University of Massachusetts (UMass) in 1947, the Metawampe Club continued its annual hike up and over Mt. Toby. In a longstanding tradition, since at least 1940, the hike has been followed by a chicken pot pie dinner at the Sunderland First Congregational Church Parish House.

Metawampe is honored on the UMass Amherst campus in the form of the bronze sculpture "Monument to Chief Metawampe" which was the class of 1950's gift to the university (shown on the cover). The statue was sculpted by Randolph Johnstone of South Deerfield using the lost wax technique. Professor Johnstone, an art professor at Smith College, taught sculpture part time at UMass in 1948 and 1949. The bronze work is 5 feet tall, weighs about 500 pounds, and is approximately three-quarters life size. In 1957, the statue was placed on a granite pedestal donated by the Class of 1956. The statue and pedestal were located within a stone and brick plaza behind the Student Union Building at the edge of the grassy area known today as the Metawampe Lawn. In 2014 as part of the Integrative Learning Center project, Metawampe was relocated 100 feet to the East, where he continues to look northward toward Mt. Toby and his ancestral homelands. In 2011 the Metawampe Statue was placed on the Inventory of Historic and Archeological Assets of the Commonwealth by the Massachusetts Historical Commission. Another Metawampe honor is the "University of Massachusetts Metawampe Fund", which was established to provide scholarships to full-time undergraduate UMass Amherst students with financial need.

The Metawampe name has been transplanted to Canada by **Chemistry Professors Howard Stidham and Thomas "Casey" Stengle**. In 1967, when they, along with others, made the first ascent of a 10,138 foot peak in the Canadian Rockies in Alberta, they christened it Mount Metawampe.

In the early 70's, the Metawampe Hike expanded to include women hikers, the first of whom was **Chemistry Professor Marion Rhodes, '66 PhD**. She was invited on the hike by **Professor Dick Stein**, former Goessmann Professor of Chemistry and Founder of the Polymer Science Department. Although the Metawampe Club and Hike started as a campus wide enterprise, over time it found a home in the Chemistry Department. Many departments have been involved over the years but the Hike continues to exist due to the organizational efforts of Chemistry Department personnel such as retired professor **Ed Voigtman**, **Professor Craig Martin**, **Professor Lynmarie Thompson**, retired professor **Dave Adams '67**, and **Bob Sabola**. The Metawampe Club today has hundreds of members since all who make the hike are indoctrinated into the club. Current officers include **Dave Adams** (president), **Bob Sabola** (treasurer), **Joe Nowicki ('92 EdD; Sociology MA '93)** (trekmaster), **Brian Konieczny (AS Stockbridge-Crop Production '84; BS Plant and Soil Sciences '95)** (spiritmaster), **Ed Voigtman**, and retired professor **Earl McWhorter** (trekmaster emeritus).

The 112th edition of the Metawampe Hike will be held November 3, 2019. So get in shape and stay hungry! The hike is four miles long and takes roughly three hours. The trail passes by waterfalls and features views of the valley from the top of the Mount Toby Fire Station. Contact Dave Adams: [adams@chem.umass.edu](mailto:adams@chem.umass.edu) for additional information and to be added to the email list for annual hike updates.

All are invited to this event which unites UMass, Chemistry, and Metawampe!



# university Engagement

## Building Bridges Art Exhibit

Building Bridges is a university-wide public art and engagement initiative designed to bring the UMass Amherst community together and foster new connections by highlighting the often hidden and diverse talents of its employees. Contributors hold a wide variety of positions on campus, representing diverse job experiences and familiarities, as well as cultural and ethnic differences. Art in its many forms is interpreted in a multitude of ways, evoking emotions and starting dialogue, so it is the perfect medium to bring about meaningful engagement. The exhibits aim to bring people together by speaking the universal language of art.

Building Bridges is one of many initiatives under the campus' larger narrative of the "Building a Community of Dignity and Respect" campaign to "...set expectations for engagement, reaffirm UMass Amherst's commitment to ensuring a safe and welcoming living-learning-working environment for every member of our community, actively build a community that honors differences, and create an environment that is respectful and inclusive for all." Building Bridges is a collaboration between the Office of Equity and Inclusion, Civic Engagement and Service-Learning, and The Partnership for Worker Education, Division of Human Resources, and other sponsors.

Campus community members were asked what differences they want to bridge and/or connect, and how they can accomplish this goal. The answers were assembled to create a mosaic for the words "building bridges." The entire campus is encouraged to include their voices each semester during the Building Bridges exhibits, and become involved through showcasing the artwork or participating in related courses.



John Donoghue and Julian Tyson

The most recent Building Bridges showcase event was held April 9 in the Fine Arts Center atrium, and featured visual arts, poetry and music from artists across campus, including art by chemistry staff members Karen Hakala, Marvin Ellin, Margaret MacDonald (retired), and music by Chemistry Prof. Emeritus Julian Tyson. Lisa Korpiewski (now in IALS) presented work and offered hands-on workshops, and as a member of the Working Group she works year round planning future exhibits. The process has created a network of new friends and valuable campus connections.



Karen Hakala's pieces were influenced by St. Jane Frances de Chantal's 'Martyrdom of Love.'



Marv Ellin: "I picked up a love of wildlife photography from my dad. It takes a lot of patience to wait for the right picture. But it is very rewarding when you are successful."

Karen Hakala: "I enjoy working with mixed media because it allows for a variety of techniques that encourage my creative side. Though I am a beginner, I find the process of doing art brings me joy and helps me better weather the stresses of life. I am particularly interested in the intersection of art and spirituality. I am grateful to artists who are staff members in the chemistry department for sharing their knowledge and inspiration."



Blue-Crowned Motmot photographed by Marvin Ellin while in Costa Rica



Watercolor Rooster by Margaret MacDonald

Lisa Korpiewski: "Mixed media art allows for a very open form of expression by building up in layers. I use paints, waxes, papers, found and handmade objects, and miscellaneous elements to create my altered art and handmade cards."

Margaret MacDonald: "The beauty of nature inspires me to paint and embrace the challenge of recreating it with watercolor."



Students in Lisa Korpiewski's workshop



## faculty Highlights

### Andrew Lab Continues to Advance the Field of Wearable Electronics

One major factor holding back the development of wearable biosensors for health monitoring is the lack of a lightweight, long-lasting power supply. Trisha Andrew and her team report that they have developed a method for making a charge-storing system that is easily integrated into clothing for “embroidering a charge-storing pattern onto any garment.”



As Andrew explains, “Batteries or other kinds of charge storage are still the limiting components for most portable, wearable, ingestible or flexible technologies. The devices tend to be some combination of too large, too heavy and not flexible.”

Their new method uses a micro-supercapacitor and combines vapor-coated conductive threads with a polymer film, plus a special sewing technique to create a flexible mesh of aligned electrodes on a textile backing. The resulting solid-state device has a high ability to store charge for its size, and other characteristics that allow it to power wearable biosensors.

One specific application the Andrew lab has made with their research is the development of pajamas embedded with self-powered sensors that provide unobtrusive and continuous monitoring of heartbeat, breathing and sleep posture — all factors that play a role in how well a person slumbers. The “smart” garments could give ordinary people, as well as clinicians, useful information to help improve sleep patterns.

“Our smart pajamas overcame numerous technical challenges,” says Andrew. We had to inconspicuously integrate sensing elements and portable power sources into everyday garments, while maintaining the weight, feel, comfort, function, and ruggedness of familiar clothes and fabrics. We also worked with computer scientists and electrical engineers to process the myriad signals coming from the sensors so that we had clear and easy-to-understand information.”

Andrew is also working with former graduate student Morgan Baima, who earned her PhD in chemistry at UMass, on a company they formed to merge technology and textiles. The company’s first product will be an innovation that’s gotten a lot of attention, including from Nike, Under Armour, and U.S. military special operations: electrically heated garments, starting with gloves made from ordinary fabric coated with super-thin conductive polymers via a process developed in Andrew lab.

### Synthetic Zeolite Research Could Be the Key to Next-Generation Biofuels

Scott Auerbach along with Wei Fan from Chemical Engineering, are combining and integrating their expertise in experimental and computational zeolite science, to shed new and important light on how zeolites self-assemble in solution, opening the door to more rational procedures for making new zeolites with advanced performance. Zeolites are the most used catalysts by weight on earth and offer the potential for 21st-century applications in carbon dioxide capture, biofuel production, and nano-electronics. Auerbach and Fan were awarded grant funds from the Department of Energy, Basic Energy Sciences in search of the “missing link” of zeolite crystallization.



Catalysts are materials that can steer chemical reactions to the most useful products, and are responsible for society’s affordable access to plastics, fuels, and other materials. Zeolites show promise for converting chemicals derived from renewable biomass into biofuels.

### Jianhan Chen Lab Discovers New Channel-Gating Mechanism and Receives New NIH Grant



Computational biophysicists are not used to making discoveries, says Jianhan Chen, Chemistry and Biochemistry & Molecular Biology, so when he and colleagues cracked the secret of how cells regulate Big Potassium (BK) channels, they thought it must be a computational artifact. But after many simulations and tests, they convinced themselves that they have identified the BK gating mechanism that had eluded scientists for many years.

BK channels are important in neuronal and muscle functions and are associated with pathogenesis of hypertension, autism, epilepsy, stroke, asthma, etc. A key puzzle has been trying to understand how cells close, or gate, BK channels, which have an unusually large central pore. “There were a lot of hypotheses, but no answers,” Chen notes. In *Nature Communications*, his team demonstrates that a phenomenon known as “hydrophobic dewetting” gives rise to a vapor phase in the pore’s central cavity to block intracellular access to the selectivity filter.

Chen’s work on BK channels has also led to a new four-year, \$2.9 million grant from NIH’s National Heart, Lung, and Blood Institute. The collaborative team includes Jianmin Cui at Washington University, St. Louis, Chen at UMass Amherst and Xiaoqin Zou at the University of Missouri.





### Gierasch Elected to National Academy of Sciences

Lila M. Gierasch, distinguished professor of Chemistry, and Biochemistry and Molecular Biology was elected by her peers to the U.S. National Academy of Sciences in recognition of her distinguished and continuing achievements in original research.

Gierasch's research focus for decades has been protein folding, that is, how amino acid sequence determines the three-dimensional structure of a protein, especially in the cellular environment and the role of molecular chaperones in ensuring high fidelity in the folding process. John McCarthy, UMass Amherst provost and senior vice chancellor for academic affairs, says of Gierasch's career accomplishments, "This is a richly deserved honor for one of our stellar faculty members. Lila Gierasch is part of what makes this university great."

Gierasch also received the 2019 Merrifield Award from the American Peptide Society to recognize her outstanding contributions to peptide science.

### Rotello Among Twelve UMass Amherst Researchers Recognized for Being Highly Cited



Vincent Rotello is one of twelve researchers at the University of Massachusetts Amherst who have been recognized for being among the world's most highly cited researchers in 2018.

The analysis by Philadelphia-based Clarivate Analytics, owner of Web of Science, serves as the basis for regular listings of researchers whose citation

records put them in the top one percent by citations for their field and year.

These scientists are judged to be "influential," and their citation records are seen as "a mark of exceptional impact," the company says. This year's list from UMass Amherst includes five more than the seven named in 2017.

### Martin 'Breakthrough' Article on RNA Synthesis

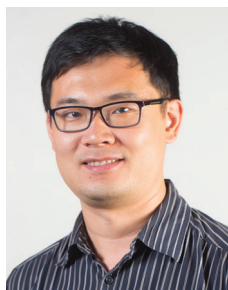


Craig Martin's lab studies the enzyme T7 RNA polymerase. This, and closely related enzymes, are used by thousands of researchers to synthesize specific RNA sequences in the test tube. New work published in the journal *Nucleic Acids Research* (and highlighted as a "Breakthrough Article") characterizes undesired (and at times, technology-limiting) errors in that synthesis, which

lead to sequences that are slightly too long or too short. Further, the work provides a mechanistic understanding that will help the design of solutions. The work exploits a modern tool in genomics, RNA-Seq, but applies it in new ways. While gel electrophoresis has been the tool of choice for the past century, this new approach represents a huge advance, identifying not just lengths of RNA, but exact sequences and sequence distributions.

RNA therapeutics companies are already taking notice, particularly those invested in mRNA therapeutics, since chemical synthesis of long RNAs is not a possibility. Impurities in the RNA trigger a potentially lethal immune response, and have been holding back major advances in what could be a key, new therapeutic approach, with wide applicability. This work does not provide the solution, but provides key understandings that may well lead to solutions.

### Mingxu You Receives Sloan Research Fellowship and NSF Career Award



Mingxu You received a highly prestigious Sloan Research Fellowship award for 2019, one of only 23 chemists nationwide to win the award this year.

"Sloan Research Fellows are the best young scientists working today," says president of the Alfred P. Sloan Foundation, Adam F. Falk. "Sloan Fellows stand out for their creativity, for

their hard work, for the importance of the issues they tackle, and the energy and innovation with which they tackle them. To be a Sloan Fellow is to be in the vanguard of twenty-first century science."

Mingxu You also received an NSF Career Award for "A Generalized Quantitative Imaging Approach for Small Molecules using Genetically Engineered RNA Sensors." You's long-term goal is to develop nucleic acid-based next-generation sensor platforms for cell biology studies and disease diagnostics. The overarching goal of his proposal is to engineer an RNA-based general sensing system for the quantitative measurement of metabolites, signaling molecules, and synthetic small molecules in living cells. These RNA-based sensors can be modularly adapted for the measurement of various analytes in individual cells, an approach widely applicable in many clinical, industrial, and ecological settings.



## Capturing Waste Heat Energy with Improved Polymers



A team led by Dhandapani Venkataraman (DV) and electrical engineer Zlatan Aksamija, reported in *Nature Communications* on an advance they outline toward more efficient, cheaper, polymer-based harvest of heat energy. “It will be a surprise to the field,” DV predicts. “It gives us another key variable we can alter to improve the thermo-electric efficiency of polymers.

This should make us, and others, look at polymer thermo-electrics in a new light.”

Aksamija explains, “Using polymers to convert thermal energy to electricity by harvesting waste heat has seen an uptick in interest in recent years. Waste heat represents both a problem but also a resource; the more heat your process wastes, the less efficient it is.”

DV and his chemistry PhD student Connor Boyle, with Aksamija and his electrical engineering PhD student Meenakshi Upadhyaya worked in what DV calls “a true collaboration,” where each insight from numerical simulations informed the next series of experiments, and vice versa. The team turned to chemist Michael Barnes, a co-author on their recent paper, who used Kelvin Probe Force Microscopy to probe the dopants at the nano level and show that clustering is indeed present in polymers doped at room temperature, but not at higher temperatures.

The findings should provide a new path for designing more efficient polymers for thermo-electric devices. DV notes that until now, chemists and materials scientists have been trying to organize polymers to be more like the inorganics, “nicely aligned and very regular, which is difficult to do,” he adds. “It turns out that this may not be the way to go; you can take another road or another approach. We hope this paper provides a basis to move polymer-based thermo-electrics forward.”

## Vachet Receives CNS Outstanding Research Award

Professor Richard Vachet was the winner of this year's College of Natural Sciences Outstanding Research Award. Richard joined the department in 1999, and he has been Department Head for the past three years. His interdisciplinary research program lies at the interface between analytical, biological and materials chemistry.

Prof. Vachet is an international leader in the field of mass spectrometry (MS). In recent years mass spectrometry has become a powerful tool in the biological sciences, where it can be used to explore the structure and dynamics of proteins. Richard and his group have developed fundamentally new ways to use MS to tackle important biomedical problems that are difficult to address with existing tools.

Prof. Vachet is best known for his work on protein amyloid formation. Soluble proteins can aggregate into insoluble amyloid fibrils, and this plays a role in many diseases, including Alzheimer's, Parkinson's and Type 2 Diabetes. It's been hard to develop effective treatments because the molecular basis for this aggregation isn't understood. Richard and his group have developed new mass spectrometric tools that provide information about protein structure during the early stages of amyloid formation. This has most recently led to the identification of molecules that can prevent amyloid formation by a protein implicated in dialysis-related amyloidosis, which affects half a million people in the US alone.

These techniques have been adapted to study protein therapeutics, which are the fastest growing segment of the pharmaceutical market. A big problem is that the 3D structure of proteins can change over time and reduce the efficacy of these therapeutic or, worse, cause unwanted immune responses. Prof. Vachet and his group have recently patented a new MS technique that can more readily detect these changes in protein structure, which has been licensed by the company QuarryBio.

Another area where Prof. Vachet and his group have made substantial contributions is in understanding how nanomaterials interact with biological systems. Nanoparticles and other nanomaterials are being developed for targeted drug delivery, particularly for the treatment of cancer. A problem with developing these treatments is that it is difficult to track and detect nanomaterials in the body. Prof. Vachet and his group have developed new mass spectrometry-based imaging techniques that can do this, and have used these techniques to determine how various nanomaterial properties modify their uptake into different cell and tissue types, facilitating the creation of better therapeutics with fewer side effects. External letter writers noted Vachet's “highly creative approaches to address highly topical research problems” and praised the breadth of his contributions.



## graduate student Accomplishments

### Riddha Das Wins People's Choice Award in Three Minute Thesis Competition



Riddha Das was one of ten finalists in this year's Three Minute Thesis Competition and won the People's Choice Award for her presentation "Nanoparticles:

New Weapons to Combat Cancer." In a general audience talk, she described her PhD research with Prof. Vincent Rotello on developing techniques to use nanoparticles to selectively deliver a protected form of an anti-cancer drug to tumor cells, and then activate the drug. This greatly reduces the harmful side effects of chemotherapy.

"It was very difficult to condense five or six years of research into three minutes," Das said, "but now if I'm at an interview or a conference, I don't have to stumble or wonder where to begin."

Organized by the Graduate School's Office of Professional Development, the annual three-week-long contest tests the research communication skills of 40 doctoral and master's students by challenging them to explain the significance of their academic projects in accessible and compelling presentations of three minutes or less.

### Francesca Anson Awarded Kuhn Fellowship



Apoptosis, or programmed cell death, maintains tissue homeostasis. Hijacking dysregulated apoptotic pathways contributing to unregulated cell proliferation is an attractive and powerful therapeutic strategy for a myriad of diseases. To utilize the potential therapeutic roles of caspases, the executioners of apoptosis, to induce cell death in a targeted

population, the Hardy and Thayumanavan labs developed a nanogel platform for intracellular caspase-3 delivery. As a joint student between the groups, and with the support of the Kuhn Fellowship I am working towards investigating caspase cargos beyond caspase-3. Further, we are exploring possibilities of caspase-nanogel and pro-survival antagonist nanogel combinatorial delivery. To maximize the potential of this synergistic platform, we are further probing caspase-nanogel conjugate self-assembly and delivery to elucidate mechanisms of cellular uptake, cargo release and potency.

### Kingshuk Dutta Wins Rausch Fellowship, Developing Methods to Deliver Therapeutics



Bio-therapeutics have gained recent momentum in the post-genomic era due to their promise in controlling human disease. Proteins, small interfering RNAs (siRNAs), enzymes, and antibodies are classical examples of biomacromolecules studied under the class of biologics. In comparison to small molecule drugs,

biologics offer higher specificity and potency with fewer side effects, leading to more predictable therapeutic outcomes. However, the dynamic and complex architecture of biologics makes them hard to stabilize in formulation and deliver to the target sites in active form. The loss of structural integrity/denaturation during systemic circulation or upon storage presents one of the major hurdles in dealing with biologics. During my graduate study in the laboratory of Prof. S. Thayumanavan, I perceived these challenges as opportunities to interrogate and design stimuli-responsive polymeric nanogel systems for the delivery of such sensitive biomacromolecules. We envisaged the possibility of encapsulating biologics through both covalent and complementary electrostatic interactions. Recently, we have successfully demonstrated intra-cellular delivery of proteins via a covalent self-immolative redox sensitive strategy by utilizing lysine moieties abundant in >85% of available proteins. Apart from designing protein delivery vehicles, I am investigating strategies for siRNA delivery that will ensure high encapsulation efficacy with low/no toxicity compared to conventional systems. In summary, the developed strategies could provide simple and robust delivery platforms potentially applicable to a broad range of bio-therapeutics.

### Kristen Sikora Awarded PPG Fellowship



Functionalized nanomaterials are attractive in applications such as sensing and drug delivery due to their tunable physical and chemical properties. My research in the Vachet lab focuses on developing novel measurement tools to monitor how the chemical and physical properties of functionalized

nanomaterials dictate their uptake and distributions in vivo. With the support of the PPG fellowship, I will be working to develop new mass spectrometry imaging methods that simultaneously monitor how nanomaterial properties affect their distributions in vivo and how these properties influence the underlying biochemistry of the biological system. Developing these methods will provide important structure/function relationships that will lead to the design of better nanomaterials for biological applications.



## new Faculty

### Philip Shivokevich



Philip Shivokevich started at UMass in the Fall of 2018 as a Visiting Assistant Professor. He received his PhD in inorganic chemistry from the University of Virginia in 2017, where he synthesized transition metal complexes with applications towards dearomatization chemistry and small molecule synthesis. After completing his degree, he spent a year teaching general, organic and

biochemistry courses as a Visiting Assistant Professor at Lander University. Philip is working in collaboration with the Knapp Group and a small team of undergraduate researchers to explore salen-type compounds for Raman-based imaging processes. He will continue to develop and update the Organic Chemistry Laboratory for Majors curriculum to meet the challenges of modern synthetic chemistry, while also teaching General and Organic Chemistry courses.

### James Walsh

Dr. James Walsh will join the UMass Amherst Chemistry department as an Assistant Professor in September 2019. James grew up in England, receiving his Master's (2010) and Doctorate (2014) degrees in chemistry from the University of Manchester. He did his PhD in the area of molecular magnetism, working with Professors David Collison, Eric McInnes, and Richard Winpenny to examine magnetic exchange interactions between highly anisotropic spin centers. Shortly after his PhD, James moved to Northwestern to work with Prof. Danna Freedman, where he helped to build the high-pressure synthesis subgroup. James will bring his expertise in high-pressure science to UMass Amherst to lead a research group investigating the effects of extreme pressure on the chemical synthesis of novel metastable solid-state compounds. He will teach majors Inorganic Chemistry and graduate Materials Chemistry. James is a big fan of autumn, and is looking forward to his first New England fall.



## faculty Retirement

### Michael J. Maroney

Mike Maroney has retired after 34 years of high profile research at UMass. His career was marked by excellence in research and teaching, including winning the University Samuel Conti Faculty Fellowship and Award for Outstanding Accomplishments in Research and Creative Activity, the CNS Outstanding Research Award, and the Lilly Teaching Fellowship. Mike's internationally renowned group produced more than 200 publications, specializing in nickel biochemistry. His work was notably creative, spanning bioenergetics, bacterial pathogenesis, metal homeostasis, and gene regulation.

Mike's work on Ni-superoxide dismutase and hydrogenases provided context for how Nickel, typically a non-redox metal, could support redox reactions. His group also made important contributions to metalloregulation, mapping out structural changes in transcription factors which discriminated amongst the bio-available metal ions. Mike mentored 20 students to successful completion of PhD degrees in Chemistry or MCB, along with numerous BS and MS researchers.

When Mike grew up in Iowa, he had no idea that his career would let him see the world. He first worked in top chemistry schools in the midwest and the West Coast, and then developing a renowned research lab in Amherst; he even spent several sabbaticals and summers working in Europe on the unusual chemistry of nickel. Mike was integral to a core group of faculty at UMass who were part rebels and part innovators, working by day to subvert the dominant paradigm and push the fore-front of science, while by night their families were tightly knit. Mike and his partners in the URC helped to create a sense of community for their colleagues in the department, which continues to this day.

Mike retired from UMass in 2018, but he remains outstanding in his field, having been elected a Fellow of the AAAS in 2015. His colleagues and students wish him the best in retirement. It is hard to imagine that he stays away for long!

- Michael Knapp



# lab Notes

## Auerbach Group

The Auerbach group had a great year in research and teaching. **Prof. Auerbach** started 2018 by going on sabbatical to study at the Swiss Federal Institute of Technology (EPFL) in Lausanne, Switzerland. In addition to skiing the Swiss and French Alps, and giving many research and education (iCons) talks throughout Europe, Prof. Auerbach also began a new sabbatical project at the Marvel National Center for Computational Materials Science on applying data science and machine learning to gain new understanding of zeolite structure and function. Back at home, Prof. Auerbach launched a new project, with major funding from the US Department of Energy, on “Integrated Experiment and Modeling of Zeolite Formation,” in collaboration with **Prof. Wei Fan** of the UMass Amherst Department of Chemical Engineering. By combining zeolite synthesis, spectroscopy, and modeling, we expect to gain unprecedented new insights into how organic molecules and silica networks conspire to



Qinfang Sun and Scott Auerbach

form crystalline nanoporous materials with a wealth of present and future applications. We look forward to reporting our latest results from this project very soon. Also very exciting was the completion of **Dr. Qinfang Sun's** dissertation work on the “Rational Design of Zeolite Clusters for Converging Aldol Condensation Reaction

Barriers.” Dr. Sun has begun a postdoc at Temple University on modeling the biophysics of protein structure and binding – we wish her well in her new field!

This has also been a terrific year for alumni of the Auerbach group. **Dr. Angela Migués** (PhD, 2016) accepted a tenure-track faculty position in the Chemistry Department at SUNY Oneonta, to begin in September 2019. **Dr. S. Vaitheeswaran** (postdoc) took a teaching position in physical chemistry at Clark University where he applied his unparalleled enthusiasm to introduce young minds to the nexus of physics and chemistry. **Dr. Hari Ramanan** (PhD, 2006) has taken a tenured position at the Indian Institute of Technology (IIT) at Tirupati, as an Associate Professor of Chemical Engineering. And perhaps the biggest news – **Dr. Cecilia Bores** (postdoc) started a family, giving birth to a son in 2018, a very productive year indeed!

We wish all alums of the Auerbach group happiness and success as they march on with their lives and professional careers. In closing, we wish all Auerbach group alums a wonderful year, and hope they'll stay in touch and visit campus whenever possible. Go UMass Chemistry!!

## Barnes Group

This year, **Prof. Mike Barnes** continued research with a collaborative grant (with co-investigators **Ashwin Ramasubramaniam** and **Todd Emrick**) from the National Science Foundation with support totaling \$450,000 (through 2021). The Barnes group also had several papers published, including a collaborative paper with **Prof. Venkataraman** (lead author) in the prestigious journal *Nature Communications* on tuning charge-transport dynamics in organic semiconductors.

**Nick Hight-Huf** is a 2<sup>nd</sup>-year graduate student in the group, and works on electric-force scanning probe techniques to probe electronic properties in hybrid organic-inorganic two-dimensional nanomaterials. **Sarah Marques** (PhD, Chemistry, 2019) will start a postdoctoral fellowship under the supervision of Carlos Silva at Georgia Tech in September 2019. **Peijian Wang** (PhD, Physics, 2018) is currently a postdoctoral researcher in the Physics Dept. at the University of Buffalo. **Joelle Labastide**, (PhD, Chemistry, 2015 “Photophysics of Semiconductor Aggregates”) was awarded a AAAS Policy Fellowship in Washington, D.C. for 2019. **Kevin Early** (PhD, Chemistry, 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, Chemistry, 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, Chemistry, 2012 “Probing Effects of Orientation on the Chiroptical Properties of Single Molecules”), is now a Microscopy and Imaging Laboratory Manager at University of Illinois-Urbana Champaign. **Ruthanne Hassey Paradise** (PhD, Chemistry, 2009, “Chiroptical Spectroscopy of Single Molecules”), is a Senior Lecturer at UMass Amherst, and supervises the Analytical and Physical Chemistry Laboratories for undergraduates.

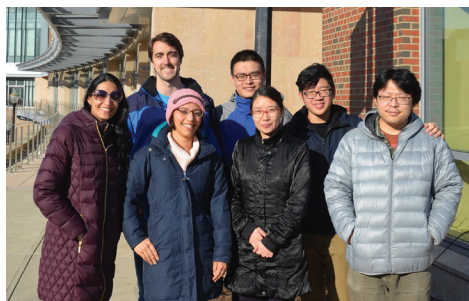
## J. Chen Group

This was another busy and exciting year for the Jianhan Chen lab. Three postdoctoral fellows, **Dr. Kuohao Lee**, **Mara Chiricotto** and **Charles English** (joint with the **Gierasch** lab) moved on to exciting new positions in academia and industry. **Dr. Azar Farjamnia**, a Visiting Researcher, relocated with her family to San Diego to become a part-time Instructor at National University. Our newly minted **Dr. Xiaorong Liu** successfully defended her dissertation in December 2018; she has remained as a postdoctoral fellow to continue working on several key projects. **Dr. Zhiguang Jia** was promoted to Senior Research Fellow in 2019. We are thrilled to welcome two new graduate students to the lab. **Erik Nordquist** hails from Idaho. He has a BS from the College of Idaho, majoring



in Physics-Mathematics and Chemistry with minors in Computer Science, History, and Philosophy! **Xiping Gong** grew up in China. He has a BS in Chemistry from Nanchang University and a MS from Xiamen University, developing density functional valence bond methods. We also welcomed **Minh Ho**, a 2<sup>nd</sup> year Biochemistry major, who came to us through the UMass STEM Ambassador program.

We have continued to make exciting progress on several active projects in the general areas of computational biophysics and biomaterials. Our research is enabled by the tremendous GPU computing capacity of our *Pikes* cluster; it is being expanded to 60 nodes thanks to an instrumentation supplement from the national Institute of General Medicinal Sciences (NIGMS) and will host 240 GPU cards! Research activities in the Chen lab were supported by a total of ~\$600K direct cost during the 2018-19 fiscal year, thanks to five active grants from NIH (3), NSF (1) and American Heart Association (1). The group has published seven original research and one editorial review article on a diverse set of topics including new molecular models, sampling method development, intrinsically disordered proteins, protein folding, ion channel



Chen lab, December 2018; Jianhan was holding the camera.

gating, and vaccine design. Our article on hydrophobic gating of BK channels is particularly noteworthy. It solves a multi-decade puzzle in the BK channel field and reveals a fascinating mechanism where ion permeation is gated by a vapor region instead of physical blockage. The work was published in *Nature Communications* and has attracted substantial attention from the field. We have also made important progress in studies of TMEM16 proteins, leading to two additional articles in *Nature Communications*. 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. Jianhan was also invited to present several departmental seminars. Group members have won several awards, including the prestigious William E. McEwen Graduate Fellowship to Xiaorong and a couple of Best Poster Awards to **Mahdieh Yazdani**.

## M. Chen Group

The Min Chen group continued to work on the functional mechanism of pore-forming membrane proteins and their biotechnological applications in biosensing.

We celebrated the graduation of two students **Christina Chisholm** and **Bib Yang** who successfully defended their

Ph.D theses. We also said good-bye to undergraduate **Gisele Andree** (BS '19) who has been working in our lab since she was a freshman in 2016! Gisele is now a PhD student in the Chemistry Department at MIT. We wish our alumni a lot of success and happiness in their career and life!



We welcome four new members: **Minji Kim**, a Food Science graduate student who is co-advised between the Chen lab and Dr. Matthew Moore's lab in the Food Science Department. She is working on building an OmpG-nanopore sensor for detecting foodborne pathogens. **Joshua Foster**, a Molecular and Cellular Biology graduate student who is experimenting on the construction of OmpG nanopore libraries for high throughput screening and selection of sensors specific for protein biomarker detection. We also welcome chemistry freshman undergraduates **Ryan Pham** and **Roy Siegelmann**.

We are grateful for a 3-year grant from the NIFA/USDA to the Matthew Moore and Chen groups to support our collaborative effort to develop OmpG-based device platforms for norovirus and enterotoxin sensing. We look forward to an even more productive year in 2020!

## Gierasch Group

This past academic year (2018-19) was a very busy one for the Gierasch lab.

As always, the lab was busy with people coming and going. We welcomed a new postdoctoral associate: **Karishma Bhasne**. Karishma came to the lab after obtaining her PhD from the Indian Institute of Science Education and Research (IISER) in Mohali, and she will study the mechanism of action of a human Hsp70 chaperone that plays a crucial role in signal transmission in neurons. We said goodbye to postdoctoral research associate **Charles English** who left the lab in 2018 and is now a Data Scientist at Impact, in New York City, as well as undergraduate student **Constantine Petridis**, who graduated as a Biochemistry major and is off to Cambridge to work at Pfizer. We wish Charles and Constantine the best of luck. Before graduating, Constantine received the BMB ASBMB award. In addition, BMB undergraduate student **Sashrika Saini** received the Jessica Hayes Scholarship, and Chemistry student **Gillian Willcox** received the Roger Bates Chemistry award for summer research (see picture on page 26). We are very proud of the successes of our lab undergraduate research students!

The lab had a fantastic year in terms of publications. We published three research articles and two major review

papers. Lila also published six editorials speaking to the readership of the *Journal of Biological Chemistry*, for which she serves as Editor-in-Chief. Happily, the paper published by former postdoctoral researcher **Abhay Thakur** and current lab member **Wenli Meng** in *Protein Science* was selected by the Protein Society as a 2018 Best Paper Award Winner. Congratulations to Abhay, Wenli, and Lila!



As usual, the group members presented their research at local meetings (including the CBI/BMB/BMP Joint Retreat, held this year at UMass Medical School in Worcester) and also traveled to other important conferences, like the Proteins Gordon Research Conference in Holderness, NH. Lila was invited to present our research at many conferences such as the Harvard Biophysics Reunion in Cambridge, MA; the CUNY biophysics symposium in NY; and the Protein Folding Disease symposium in Ann Arbor, MI. Importantly, she traveled to Monterey, CA to the American Peptide Symposium where she received the prestigious 2019 Merrifield Award by the American Peptide Society in recognition of a lifetime achievement in the field of peptide science.

Happily, the lab welcomed two new baby girls to the Gierasch family: postdoc **Sasha Pozhidaeva**'s baby Danica was born in November, and postdoc **Wenli Meng**'s daughter Chloe was born in May. All are filled with joy and we wish them the very best.

Recently, two very big events made this year perfect for the lab. First, Lila was elected to be a member of the National Academy of Sciences. The whole UMass community (and more) are very proud of Lila's well-deserved achievements. Second, last May the Gierasch lab celebrated 45 years of life (and success) with an alumni reunion. More than 60 people who were members of the lab at various times since the lab started in 1974 at Amherst College gathered at UMass Amherst where we enjoyed a one-day symposium. People came from all over the world (Turkey, Poland, France,

Germany, all over the US, and more!) and presented short talks where they shared their scientific work as well as memories from their lab days. We ended the evening with dinner and a dance party. It was a fantastic event, and we all celebrated being part of the Gierasch Lab family.

We are geared up for another year of great success!

## Hardy Group

The Hardy Lab has continued to enjoy success in the past year. In September 2018 **Prof. Jeanne Hardy** was promoted to the rank of Full Professor, thanks to the more than a decade of awesome work by the talented group of students and postdocs she has been fortunate to mentor. She was also invited to serve as Master of Ceremonies for the opening of the MassBio West office, which included introductions of dignitaries including **US Congressman Richard Neal**, Chair of the House Ways and Means Committee, and **Chancellor Subbaswamy**. This year the Hardy Lab saw several members complete their training, and welcomed new students in their stead. In September both **Maureen Hill** and **Derek MacPherson** successfully defended dissertations. Maureen's work on Zika virus protease was published in *ACS Chemical Biology* and in *ACS Biochemistry*. Derek's work describing a new exosite in caspase-6 was published in *The Journal of Biological Chemistry*. Maureen has gone on to a scientist position at FOG Pharmaceuticals and Derek is working for Silicon Therapeutics utilizing the skills in hydrogen-deuterium exchange he gained at UMass. Undergraduate researchers **Christopher Chinman** (Chemistry) and **Amber Colon** (Chemical Engineering) both received their baccalaureates in the May 2019 commencement.

With so many successful PhD defenses in the recent past, we were delighted to welcome three fabulous new graduate students, **Sparsh Makhaik** (University of Delhi and JAIST), **Irina (Niña) Sagarbarria** (University of the Philippines Los Baños), and **Andrew Smith** (Stony Brook University). All three are off to a fabulous start, developing new projects on emerging viral proteases, determining the structure of inhibited caspase-6 and discovering new caspase-6 exosites. **Ishan Soni**, a CBI fellow, co-authored a collaborative paper with ActivX BioScience Inc that was published in *ACS Biochemistry* on the functional implications of caspase-6 regulation by various nucleotides. **Francesca Anson**, who this year completed her BTP fellowship including a pharmaceutical internship at MedImmune, was awarded the highly coveted top poster prize at the 2019 UMass Amherst CBI-UMMS joint retreat for her collaborative work with the **Thayumanavan** lab on caspase delivery. **Kristalle Cruz** successfully defended her prospectus and began work on two new alphaviral proteases. This year we also welcomed two new undergraduate researchers, **Ethan Goulart** (Chemistry, CHC) and **Justin Baker** (BMB, CHC) to the lab.



This year we extended the tradition of a Hardy Lab ski trip (photo below) to the entire department and hope to see



even more skiers and snowboarders next year! Because we are always hoping for additional Hardy Lab skiers, we were thrilled to hear that

alumnus **Kristen Huber** (PhD 2012; Signum Biosciences) welcomed a new daughter, Melody Skye Wilson. Alumnus **Witold Witkowski** (PhD 2011) moved to a new position at Quest Diagnostics to focus more on big data science. **Dee Lin** (BS 2013) completed Pharmacy school and started a new job at Janssen as a manager in health economics and outcomes research. Overall, Hardy lab alumni are making great impacts in industry, academia, and the military, and we are very proud of their accomplishments.

## Jackson Group

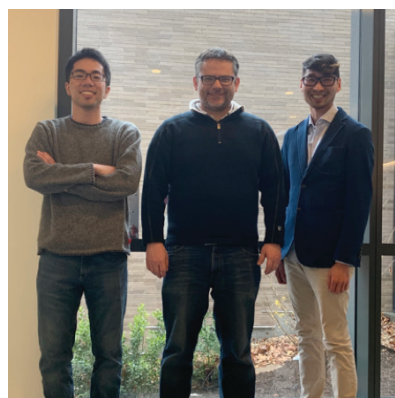
The Jackson group continues to explore the dynamics of methane dissociation on transition metal-based catalysts. This is the rate-limiting step in the steam reforming of natural gas. We have developed quantum mechanical methods that allow us to compute the dissociative sticking probability of methane as a function of the translational energy and vibrational state of the methane molecule, as well as the temperature of the metal. Graduate student **Han Guo** has been examining  $\text{CH}_4$  reactions on stepped Ni(211) and Pt(211) surfaces. It has long been suspected that the reactivity on “real” catalysts is dominated by reactions at step edges and other defect sites. We have shown that this is so, in collaboration with an experimental group at EPFL (Lausanne, Switzerland). In Han’s most recent paper she was able to fully resolve these methane reactions, under typical reactor conditions, in terms of surface impact site, collision energy, methane vibrational state, and the thermal motion of the lattice. This work, published in *Journal of Chemical Physics*, was selected as an “Editor’s Pick” and promoted on the journal homepage. Han successfully defended her PhD thesis in August of 2018. Prof. Jackson will present this work in a Keynote Lecture at the Frontier Science symposium, *Molecules at Surfaces: What Do We Really Know?*, in Liverpool, UK, and at the *Spectroscopy and Dynamics of Molecules and Clusters* meeting in Rajasthan, India.

## Kaltashov Group

2018 was a very busy year in the Kaltashov laboratory, which included publication of ten peer-review papers, as well as several presentations given by group members at numerous scientific meetings and conferences. The group’s research programs were supported by the National Science Foundation and the National Institutes of Health (NIH). A new NIH grant was also awarded in spring 2019 to develop new analytical techniques that integrate chromatographic separations with in-line chemical reactions to study complex biological macromolecules. The group has also completed contractual work (with Sentier Therapeutics) to study thyroglobulin, the natural source of levothyroxine, the number one prescription medication in the United States. **Jake Pawlowski** defended his PhD dissertation and moved to Amgen (Cambridge, MA), and a new graduate student, **Daniel Favre**, joined the group in December 2018.

## Kittilstved Group

The past year featured interesting science discoveries in the realm of inorganic materials chemistry at UMass and some exciting changes in the Kittilstved Group. Following the group’s move to the first floor of the new Physical Science Building in July 2018, we also celebrated the tenure and promotion of Kevin in September. It is a great testament to the genuine curiosity and hard work of the current and former graduate and undergraduate students that



Fumi Kato, Kevin, and William Harrigan

made this personal accomplishment possible. We started the academic year with six graduate students and finished the year with two more successful PhD defenses by **Dr. Fumitoshi Kato** (“Synthesis of Transition Metal Ion Doped Metal Benzenechalcogenolate Clusters”) and **Dr. William Harrigan**

(“Modulating Dopant-Defect Interactions in Transition Metal Doped Colloidal Strontium Titanate Nanocrystals”). The group wishes these members all the best.

The four remaining graduate students in the group (**Enes Buz**, **Jillian Denhardt**, **Haneen Mansoor**, and **Abdullah “AB” Muhammad**) have very been productive in the lab. In addition, Jill, Haneen and AB all passed their exams to become official PhD candidates and Enes passed his Prospectus! This summer, AB will attend a competitive summer school and present a poster at a conference in Denver on electron paramagnetic resonance (EPR)

spectroscopy. For more highlights from the group and to see the latest news from the Multifunctional Inorganic Materials Chemistry (MIMC) lab, please check out our website <https://mimclab.umasscreate.net> or follow us on Twitter (@mimclab)!

## Knapp Group

**Vanessa Chaplin** defended her thesis, focusing on the facial triad of FIH-1, then moved to start her ORISE postdoctoral fellowship at the Naval Medical Research, San Antonio, TX—Congratulations! **Mike Mingroni** is continuing his research on metal sequestration and hypoxia, and is wrapping up a study on intramolecular isotope effects. **Ran Duan** completed his prospectus on SERS detection of hypoxia, and is making excellent progress. **Isabella Jaen Maisonet** continued her undergraduate research on HIF hydroxylases, and has taken a summer fellowship with the BCMP Summer Scholars program. Isabella received the William Bulger Presidential Scholarship, and was selected as an ACS Scholar – way to go! **Prof. Philip Shivokevich** started as visiting Assistant Professor, and led research in the lab on ZnSalen fluorescence with two undergraduates, **Julianna DiRenzo** and **Mitchell Buckley**.

## Martin Group

Last Fall, **Yasaman Gholamalipour** and **Aruni Karunanayake Mudiyansele**'s paper using RNA-Seq as an analytical tool to derive mechanism in transcription was selected by the Editors of *Nucleic Acids Research* as a "Breakthrough Article." The work was presented last year at the Annual Meeting of the RNA Society, the RNA Therapeutics Conference, and the mRNA Health Conference. You might guess from this that the paper has some important applications. Indeed, it has launched us in a new direction, using mechanistic understanding to design better ways to make RNA. Together with undergraduate **Will Johnson**, she has a second manuscript under review at *Nucleic Acids Research*, this one focusing on a specific new approach which significantly increases both yield and purity in RNA syntheses by T7 RNA polymerase.

**Elvan Cavac** and **Kithmie Malagoda Pathirana** have been developing powerful new approaches towards synthesis and Elvan recently traveled to Krakow, Poland to present our work at the 2019 Annual Meeting of the RNA Society. Kithmie and Yasaman will be presenting our lab's work at the 2019 RNA Therapeutics Conference, much closer in Worcester, MA.

Undergraduates **Kira Chandran**, **Adrian Radel**, and **Kyle Koczera** completed their Honors Theses this year and are off

to new vistas: Kira to medical school at Georgetown, and Kyle to graduate study in Chemistry at Ohio State.

The MartinLab has a new web site at <https://martinlab.chem.umass.edu/> (featuring a new crowd sourcing campaign!) and a new @martinlabchem social media presence on Twitter. Please check us out, RT us, and if you haven't, connect with us through LinkedIn.

## Metz Group

The Metz group has had an exciting year exploring the interactions between transition metal ions and small hydrocarbons and studying the photodissociation dynamics of metal-containing ions. We welcome graduate student **Apakorn Phasuk** to the group! Graduate student **Justine Kozubal** and undergraduate **Tristan Heck** have been studying interactions between early transition metal cations and one to several methane molecules. In an exciting development, they observed C-H activation by  $Zr^+$  and used vibrational spectroscopy to determine the structures of the reaction products. We greatly enjoyed having **Prof. Jesse Marcum** (Framingham State University) work with our group during his sabbatical this Spring. He studied complexes of  $V^+$  with ethane using experiment and theory, showing how internal rotation of the ethane affects the C-H stretches. Second-year graduate student **Schuyler Lockwood** is using photofragment imaging to study the products, anisotropy and kinetic energy release in photodissociation of  $MgI^+$ , observing selective formation of  $Mg^+$  or  $I^+$ , depending on the photodissociation wavelength. We just received an NSF grant to study interactions of transition metal cations and cluster cations with ethane and propane, and to use photofragment imaging to study photodissociation dynamics in polyatomic molecules.

**Prof. Metz** presented these results at the Gordon Conference on Gaseous Ions and at the Molecular Interactions and Dynamics Gordon Conference, where he was elected vice-chair for the 2020 meeting. In alumni news, **Chris Copeland** (PhD, 2017) recently started a new job as a senior associate scientist in the Drug Metabolism and Pharmacokinetics team at Cycleron Therapeutics Inc. and Michael "Dave" Johnston (PhD, 2018) has returned to his alma mater, The College of Charleston, to be their laboratory instrument and electronics technician. Please send a note to let us know how you're doing, or just stop by if you're in the area!

## Rotello Group

Vince has done quite a bit of traveling, with plenary talks in the US, Scotland, and Thailand. He was also honored as a Highly Cited Researcher by Clarivate/Web of Science. The publication total is ticking up, with the current count at 570.



The group has new funding from the NIH for wound biofilm research (in collaboration with **Robin Patel** at the Mayo clinic), along with a new grant from the NSF in collaboration with the **Vachet** group.



**Riddha Das** and **Akash Gupta** both won the Scholarship Award from GRC chairs during the Gordon Research Conference held at Vermont last August. Three of our group members—**Sanjana Gopalakrishnan**, **Riddha Das** and **Akash Gupta**—won the Outstanding Poster Award in the Colloid and Surface Chemistry Division during 256th ACS National Meeting & Exposition in Boston. At ResearchFest 2018, **Sanjana Gopalakrishnan** and **Jessa Marie Makabenta** won the Dr. Paul Hatheway Terry Award for Outstanding Poster Presentation while **Akash Gupta** bagged the Marvin D. Rausch Scholarship Award for Outstanding Oral Presentation. **Riddha Das** won two more awards: People's Choice Award during the recent #UMass3MTFinals; and Best Poster Award at the Supramolecular Biomaterials for Regenerative Medicine and Drug Delivery Poster Session during the recently concluded 2019 MRS Spring Meeting and Exhibit in Phoenix, Arizona. Moreover, the research article by Huma, Gupta et al. was recognized as the ACS Editors' Choice from *ACS Omega* last December.

In addition, our group hosted a field trip for middle and high school students from Commonwealth Academy in Springfield. The students were toured around the Light Microscopy Core Facilities in the Life Sciences Laboratories, and the Transmission (TEM) and Scanning (SEM) Electron Microscopes in the Conte Polymer Research Center. Vince enthused the students in his talk on the use of nanomaterials as antimicrobials. And for a more hands-on experience, graduate students demonstrated experiments on growing bacteria, preparing an essential oil-based emulsion, and eradicating bacterial biofilms—which some of the students got to try themselves. The day's event was organized and coordinated by Akash Gupta.

On the departure side, **Ryan Landis** and **Li-Sheng Wang** received their PhDs, with Ryan joining Translate Bio and Li-Sheng to Rensselaer Polytechnic Institute. The group bid farewell to Postdoctoral Fellows, Visiting Professors and Visiting scholars: **Dr. Xinhong Chen**, **Morgane Malassine**,

**Loic Herter**, **Jade Caillieaudeaux**, **Marie Hattstatt**, **Sawinee Ngerpimai**, **Yagiz Anil Cicek**, **Dr. Jing Yang**, **Dr. Federica Scaletti Acciai**, **Jiadi Sun**, **Dr. Joseph Adeyemi**, **Dr. Xuewen Wu**, **Dr. Roberto Cao-Milan**, **Shichao Lin**, **Muhammad Usman**, **Dr. Shumei Zhai**, **Jessica Kretzmann** and **Lucrezia Ferracuti**. We have had a strong influx of new faces including **Aritra Nath Chattopadhyay**, **Ritabrita Goswami**, **Aarohi Gupta** and **Ahmed Nabawy** who have officially joined our group as graduate students. Welcome to the group!

## Thayumanavan Group

It's been an exciting year for the Thayumanavan Research Group in our new home on the second floor of the Physical Sciences Building. Below are a few of the highlights.

On June 1-June 2, we welcomed group alumni back to UMass Amherst for the 20<sup>th</sup> Reunion of the Thayumanavan Research Group! In addition to our current research group members, those attending were: **Dr. Diego Amado-Torres** (Pall Corporation), **Dr. Sivakumar Aathimanikandan** (Albany Molecular Research), **Dr. Malar Azagarsamy** (Partikula), **Dr. Youngju Bae** (University of Massachusetts Lowell), **Dr. Subhadeep Basu** (Lam Research Corp.), **Dr. Pandi Bharathi** (Cambrex Pharma), **Dr. Krys Bronk** (Ingevity), **Dr. Jing Guo** (IBM Research), **Dr. Huan "Joy" He** (DuPont), **Dr. Longyu Li** (Dartmouth College), **Dr. Bhooshan Popere** (DuPont) **Dr. Raghunath Roy** (Dow), **Professor Ja-Hyoung Ryu** (UNIST, South Korea, currently doing a sabbatical year at Brandeis University), **Dr. Elamprakash Savariar** (Vertex Pharmaceuticals), **Dr. Velu Sivanandan** (Seo Corp.), **Dr. Judy Ventura** (Nitto Avencia), **Dr. Feng Wang** (Global Foundries), **Mr. Dongsik Yang** (Brandeis University), **Dr. Bo Zhao** (University of Mass.) Some people also brought their families and it was wonderful to see all the kids.

The two days were filled with talks (both by current group members and alumni), much reminiscing, career advice by alums for the current students and a discussion of the future directions of the Thayumanavan Research Group. Each alum received a memento of the occasion — a framed photo of everyone who attended. Many attendees and also alumni who



were unable to attend sent powerpoint slides that included a variety of entertaining and hilarious photos from their time in the lab.

Prof. Thai and his wife, Sharmila, hosted a BBQ at their home on Saturday evening, giving everyone a chance to socialize and enjoy some great food. We owe a special thanks to them and the Social Committee of the research group working in concert with Dr. Pandi Bharathi, for putting this wonderful event together!

This year, **Ritam Das**, **Shuai Gong**, **Uyen "Jenny" Huynh**, **Pintu Kanjilal**, and **Stephanie "Steph" Le** were welcomed as new graduate students in the group. Current graduate students, **Kingshuk Dutta** and **Khushboo Singh**, are both participating in internships this summer. Kingshuk's internship is with Merck & Co. in Pennsylvania. Khushboo's is with Vertex in San Diego. In addition, Kingshuk was awarded the Marvin D. Rausch Fellowship. **Francesca Anson**, a joint student with the Hardy Lab, was awarded the Kuhn Fellowship (see page 9).

## Thompson Group

Congratulations to **Dr. Maryam Kashefi** who defended her thesis in December 2018. Maryam moved in February to sunny San Diego where she is doing a postdoc with Galia Debelouchina at UC San Diego, using NMR and other biophysical methods to investigate the phase separation of proteins involved in neurodegenerative disease. Congratulations also to **Dominique "Kiki" Carey** who graduated in May with a BS in Chemistry. This summer Kiki will start a position as a Research Associate in the Proteomics Platform at the Broad Institute in Cambridge, MA.

We are happy to welcome to the lab Chemistry graduate student **Katie Wahlbeck**, MCB graduate student **Thomas Tran** and undergraduate Biology major **Brianna Manning**. We also hosted undergraduate **Seth Cowan** from Penn State Behrend for summer research as part of the CURE program, to work on a collaborative project with the **You** lab, to use RNA nanostructures for ligand-controlled assembly of chemoreceptor arrays that could ultimately be used for bioremediation.

Congratulations to Kiki Carey, who received the Sir Harold W. Kroto and Steve F.A. Acquah GEOSSET Award, and to **Tiernan Kennedy**, who received the ACS Membership Award and Tarselli Family Research Award. Tiernan also won an award for his poster at the Chemistry undergraduate poster session in April. And, last but not least, congratulations to Katie Wahlbeck who was awarded a CBI Traineeship to start in September 2019.

Lynmarie enjoyed participating in an outreach activity at the intersection of art and science: Pipettes and Paintbrushes

(<http://thatlifesci.com/Events/>). Lynmarie described the beautiful hexagonal symmetry and the interplay of order and flexibility in chemotaxis receptor arrays to her partner, Science and Engineering librarian and UMass alumna **Melanie Radik**. What a cool origami model Melanie created of the array!



Summer 2018 was a busy one, with Lynmarie co-organizing the Molecular Biophysics of Membranes FASEB conference, where Maryam spoke, Maryam also presenting her work at the Protein

Society meeting in Boston, and Lynmarie, Aruni, and Nikita attending the chemotaxis-focused Receptorfest at Cornell. We were proud to have **Amber (Yael) Balazs** (PhD 1999) be the keynote speaker at Researchfest at the end of the summer.

In January, **Aruni Karunanayake Mudiyanse** presented her interesting HDX-MS results on the kinase controlled by chemoreceptors at the BLAST (Bacterial Locomotion and Sensory Transduction) meeting in New Orleans. In April, Lynmarie and **Nikita Malik** attended the ENC (Experimental NMR Conference) in Asilomar, CA and presented our findings on signaling-related changes in dynamics in chemoreceptors. The lab is excited that our recent HDX-MS and NMR results have led to a novel hypothesis for how receptors transmit signals 200 Å: we propose that functional chemoreceptors have a partially disordered cytoplasmic domain, and signaling inputs modulate that disorder to alter binding contacts and activity of the kinase they control. Finally, Lynmarie enjoyed attending ABRCMS (Annual Biomedical Research Conference for Minority Students) in November 2018 in Indianapolis. It was inspiring to meet so many talented students and participate in a meeting that is completely focused on promoting student success!

## Vachet Group

Research in the Vachet group continued in the areas of protein amyloid formation, detection of nanomaterials in cells and tissues, biomarker detection by mass spectrometry, and methods to monitor the structural integrity of protein therapeutics. The group was productive, despite Richard serving his third year as Department Head, publishing 12 papers on these topics in 2018 and the first few months of 2019. Professor Vachet and his group made close to 20 presentations at various conferences, meetings, and universities. Richard was also awarded the College of Natural Sciences Outstanding Research Award for 2019 (see page 8).



In group news, we said good-bye to three students. **Mahalia 'Mac' Serrano** successfully defended her PhD in September 2018 and is now working at Bristol-Myers Squibb in New Jersey; **Bo Zhao** defended his PhD in May 2019 and is headed to AbbVie in Worcester, MA; and **Tyler Marcinko** was the first MCB student to finish his PhD in the group, also successfully defending in May 2019.

We welcomed three new graduate students into the group – **Stacey Nash** (an MCB student), **Dheeraj Agrohia**, and **Zachary Kirsch**, who received his BS in Chemistry at UMass and decided to stick around Amherst for grad school. Stacy will be studying pre-amyloid oligomers of  $\beta$ -2-microglobulin, Dheeraj will be developing some new mass tags for tracking and imaging polymeric drug delivery agents, and Zack will use covalent labeling/mass spectrometry data to improve protein structure prediction by computational methods.



In alumni news, some former students transitioned into new jobs. **Adam Graichen** (PhD 2012) is now the manager of the mass spectrometry facility at the University of Connecticut. **Bo Yan** (PhD 2014) took a new position at Beam Therapeutics in Cambridge, MA, and he also got married in March! Congrats Bo! **Jia Dong** (PhD 2014) also welcomed her son Miles Everett Liu into the world this past Spring. Congrats Jia!

## Venkataraman Group

The Advanced Laboratory for Iontronic, Electronic, and Nanomaterials (ALIEN) a/k/a the DV Group had a great 2018-2019 academic year. The DV Group is now 20 years old! A big and heartfelt thank you to all the DV group alumni who contributed to the foundation and growth. Last August, we moved to the brand new Physical Sciences Building. As we cleaned out the LGRT labs, we reminisced on some of the memorable events on the 15<sup>th</sup> Floor.

**Christie Ellis**, a graduate student, received a 2018 AAAS MassMedia Fellowship and worked as a summer intern at the St. Louis Dispatch. This fellowship allowed Christie to learn about communicating science to a broader audience. **Emily Smith**, also a graduate student, received the CNS Teaching Fellowship, and she will develop a new course for Freshmen

in the fall. **Connor Boyle** and **Seung Pyo Jeong** received their PhDs. Connor's dissertation probed the impact of dopants in conjugated polymers on the thermoelectric properties of the polymers a new direction for the DV group. Seung Pyo completed his studies on polymeric materials for high energy density photo-thermal batteries. We took some of the ideas from his work and have started to collaborate with a colleague in Kinesiology on power muscle Myosin using abiotic molecules. Yeah, you are reading it right. DV group now has a bio-related project! After his graduation, Connor took a position at Bard College in New York City. He is currently teaching in the Baltimore area, where his wife is doing her internship. Seung Pyo is now a postdoctoral associate at Oak Ridge National Laboratory in Tennessee.

The DV group welcomed **Michael Lu-Diaz** as a new graduate student, who will build on the foundation laid by Connor. Michael also received the Smith-Spaulding Fellowship from the UMass Amherst Graduate School. **Eric Ostrander** joined the group as a visiting scholar and developed key abiotic molecules for powering muscle myosin. Eric will become a first-year graduate student in the Fall. We also welcomed several excellent undergraduate researchers: **Sam Stroup**, **Sam Knight**, **Alex Amato**, **Benjamin Frick**, and **Justin Blundell**. Sam Stroup received the Department Chemistry Research Award and is the first freshman to receive this award. Sam Knight received the Shapiro Award for academic excellence.

From the alumni side, **Matthew 'Donnie' Rollings** received an NSF Doctoral Fellowship. He is a graduate student at the University of California at Berkeley. **Julia Lenef** is pursuing her graduate studies in Materials Science and Engineering at the University of Michigan Ann Arbor. **Derek Van Allen** (PhD

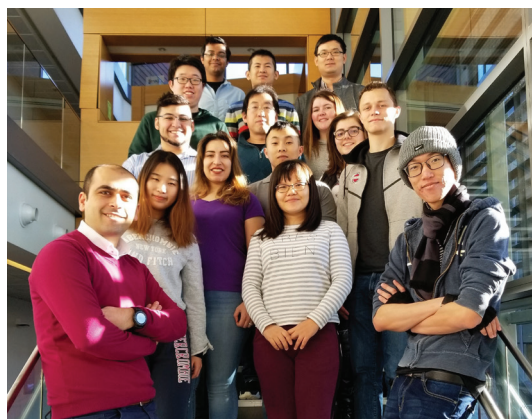


'04) was a panelist in the Researchfest Alumni panel in our Department. He came back in the Fall to recruit UMass students for Pratt and Whitney. We hope to have more alumni return to UMass and recruit our students. **Sravan Surampudi** is now officially a lecturer in our department. **Tim Gehan** (PhD '16) took a new job at Tandem PV, a start-up out of NREL. **Rattan Gujadhur** (PhD '03) started his own company, Nutri-Innov Pharmaceuticals. 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](mailto:dv@umass.edu). For group updates and news, visit us on the web at [thedvgroup.com](http://thedvgroup.com) and follow us on twitter @dvgroupumass or on Instagram: dvgroup\_umass.

## You Group

This is our third year here at UMass, and it has been a busy but fruitful year. In February, **Prof. Mingxu You** received a five-year NSF CAREER Award to support development of genetically encoded RNA-based sensors. In the same month, he was selected as a Sloan Research Fellow in Chemistry. This two-year fellowship recognized 23 early-career chemists with outstanding promise nationwide. Moreover, Prof. You has been selected as an Emerging Supramolecular Chemist in North America by the journal *Supramolecular Chemistry* and as an Emerging Investigator by the journal *Analytical Methods*. He also joined the editorial board of *PeerJ Analytical Chemistry*.

This year we have published seven manuscripts, with two more under review. **Aruni Karunanayake Mudiyanselage**, a research fellow in the lab, published in the *Journal of the American Chemical Society* with a highly sensitive way for imaging low-abundance RNAs in live cells. **Qikun Yu**, a third year graduate student, described a novel RNA-based sensor for intracellular imaging of silver ions in *Chemical Communications*. In another work published in *Cell Chemical Biology*, Prof. You and **Rigumula Wu** demonstrated the detection of low amount metabolites in live cells using a novel RNA ribozyme-based sensor. These works have been partially supported by our recently granted National Institutes of Health (NIH) proposal to understand the mechanism of antibiotic resistance.



A new postdoc, **Dr. Kewei Ren**, and two graduate students, **Puspam Keshri** and **Qian Tian**, joined the lab this year. An MS student, **Manojkumar Narayanan**, from UMass Lowell joined the lab for his thesis research. As part of the CURE-REU program, an undergraduate from UT Austin, **Nicholas Fong**, joined the lab for summer research. Rigumula Wu, **Yousef Bagheri** and **Qikun Yu** have passed the original research proposal defense and become PhD candidates. On the departure side, several undergrads in the lab, **Mark Leon-Duque**, **Sara Chedid**, **Yeonsoo Kum**, and **Tony Nguyen** have graduated from UMass or Mt. Holyoke College. We will miss all of you!

Lab members have also received several awards. A seed grant from the Institute of Applied Life Sciences (IALS) was awarded to support our development of probes to study transient membrane interactions. Graduate students Yousef and Qikun received departmental travel grants. Qikun also received a CBI travel grant. Yousef received funding to attend a week-long Quantitative Fluorescence Microscopy course in Maine and was also awarded a William E. McEwen Fellowship Award for his outstanding poster presentation during ResearchFest 2018. Our undergrads have also been recognized by several awards, including Mark Leon-Duque receiving the UMass Amherst Rising Research Student Achievement Award.

Many group members presented at PITTCON 2019 in Philadelphia. Prof. You also gave an invited lecture on DNA/RNA nanotechnology in INSERM, an equivalent of NIH in France. In addition, Qikun presented in the five-college Pioneer Vallege "RNA Salons". **Dr. Bin Zhao** and Rigumula Wu represented the group by giving a CBI Chalk Talk. Moreover, Prof. You organized a two-day *Nucleic Acid-based Sensors* Symposium at the 256<sup>th</sup> ACS National Meeting in Boston. He also organized a CBD *Nucleic Acid Delivery* Workshop at UMass.

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

### Additional Faculty Notables

**Lara Al-Hariri** was awarded a Senior Lecturer Professional Improvement Fellowship for Fall 2019.

**Trisha Andrew** was selected to present the Kavli Foundation Emerging Leader in Chemistry Lecture at the ACS National meeting.

**Jianhan Chen** received NSF funding to study 'Floppy' Proteins, a class of proteins with highly flexible three-dimensional structural properties.

**S. "Thai" Thayumanavan** received the Distinguished Graduate Mentor Award from the UMass Graduate School.

**Lynmarie Thompson** (joint PI) was awarded an NIH grant to continue supporting the Postbaccalalaurate Research Education Program (PREP), which supports educational activities that enhance biomedical, behavioral, and clinical research workforce diversity.

**Gabriela Weaver** has been named American Council on Education Fellow for 2019-2020.



# 28th annual ResearchFest

The 28th annual research symposium, ResearchFest, welcomed the incoming first year students last August with the keynote address given by **Dr. Yael Amber Balazs** (Thompson lab '99). The event was a huge success thanks to the support of participants, organizers, and sponsors, and featured six oral presentations by graduate students who were selected by a faculty committee through a nomination/evaluation process.

The **Marvin D. Rausch Scholarship Award** for Outstanding Presentation was awarded to **Akash Gupta** (Rotello group) for his work on "Engineering Nanomaterials for Imaging and Therapy of Bacteria and Biofilm-Associated Infections" and **Jingjing Gao** (Thayumanavan group) received the **William E. McEwen Graduate Scholarship in Chemistry** as runner up for her work on "Supramolecular Assemblies for Protein Transport Across Solvent Interface."

Four finalists received **William E. McEwen Awards** for their presentations: **Hui-Hsien "Tanya" Lin** (Farkas Group), **Patanchai "Kong" Limpikirati** (Vachet Group), **Xiarong Liu** (J. Chen Group), and **Kirandeep Deol** (Strieter Group).

Over 60 graduate students presented posters, and **The Dr. Paul Hatheway Terry Awards** for Outstanding Poster Presentations were presented to **Sanjana Gopalakrishnan** (Rotello Group), **Bishnu Joshi** (Farkas Group), and **Jessa Marie Makabenta** (Rotello Group).

Four students received the **William E. McEwen Fellowship Award** for Outstanding Posters: **Francesca Anson** (Hardy/Thayumanavan Group), **Yousef Bagheri** (You Group), **Thameez Mohammed K Y** (Thayumnavan Group), and joint poster **Peidong Wu/Khushboo Singh** (Thayumanavan Group).

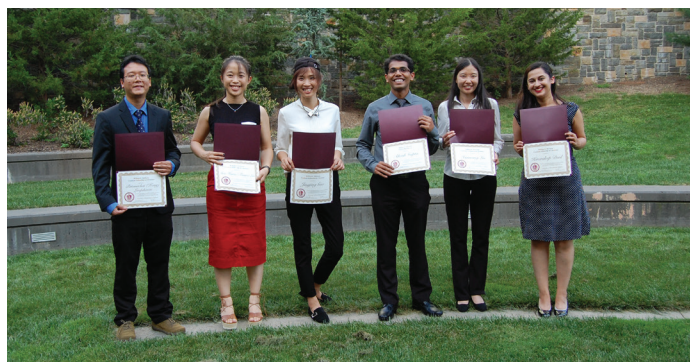
The Association for Professional Development in Chemistry (APDC) held a cookout in the amphitheater behind the ISB for students, faculty, staff, and their families.

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. We also thank the following vendors who came to show us what their companies had to offer: ThermoFisher Scientific, Eppendorf, Beckman Coulter, Chemglass Life Sciences, IKA, Thermo Scientific, and General Electric Healthcare.

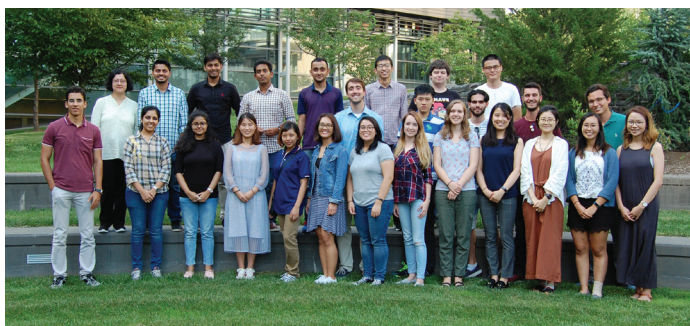
If you are interested in contributing to this event, please contact Vicki Hubby at [vicki@chem.umass.edu](mailto:vicki@chem.umass.edu).



Poster winners (left to right): Yousef Bagheri, Jessa Marie Makabenta, Sanjana Gopalakrishnan, Bishnu Joshi, Thameez Mohammed K Y, Francesca Anson, Khushboo Singh, Peidong Wu



Talk Award Winners: Patanachai "Kong" Limpikirati, Hi-Husien "Tanya" Lin, Jingjing Gao, Akash Gupta, Xiaorong "Sharon" Liu, Kirandeep Deol



Incoming Fall 2018 Graduate Students: Ahmed Nabawy, Sparsh Makhaik, Aarohi Gupta, Pintu Kanjilal, Ritabrita Goswami, Dheeraj, Qian Tian, Ritam Das, Apakorn Phasuk, Aritra Chattopadhyay, Irina Sagarbarria, Erik Nordquist, Kaitlyn Chhe, Tongkun Wang, Anastasiia Komarova, Shuai Gong, Daniel Favre, Katie Wahlbeck, Andrew Smith, Xiping Gong, Fangying Huang, Zachary Kirsch, Ruolan Fan, Stephanie Le, Michael Lu-Diaz, Uyen Huynh. Not pictured: Reza Avazzadeh, Maryam Shahryari



Prof. Richard Vachet with Kathy and Don Schulz



APDC cookout behind the Integrated Sciences Building



# PhD degrees

Awarded May 2018 - May 2019

**Morgan Baima**, *"Surface Functionalization of Fabrics and Threads for Smart Textiles,"* Trisha Andrew

**Connor J. Boyle**, *"Impact of Chemical Doping on the Thermoelectric Charge Transport of Organic Semiconductors,"* D. Venkataraman

**Vanessa D. Chaplin**, *"Role of the Facial Triad in Factor Inhibiting HIF (FIH): Ligand Binding, Substrate Selectivity, and Uncoupling,"* Michael J. Knapp

**Fatih Comert**, *"Precipitation and Coacervation in Polyelectrolyte-Colloid Systems,"* Richard W. Vachet & D. Venkataraman (post-Paul Dubin)

**Han Guo**, *"The Dissociative Chemisorption of Methane and Its Isotopologues on Metal Surfaces,"* Bret Jackson

**William L. Harrigan**, *"Modulating Dopant-Defect Interactions in Transition Metal Doped Colloidal Strontium Titanate Nanocrystals,"* Kevin R. Kittilstved

**Maureen E. Hill**, *"Active Site Design and Exploitation of Allosteric Sites in Proteases,"* Jeanne A. Hardy

**Hsin-Ting "Tiffany" Huang**, *"Nickel Site Structure and Function in Biological Sensing and Enzyme Activity,"* Michael Maroney

**Seung Pyo Jeong**, *"Azobenzene-based Polymers for Organic Electronics and Photo-Thermal Batteries,"* D. Venkataraman

**Maryam Kashefi**, *"Chemoreceptor Dynamics and Signaling: NMR Measurements within Functional Complexes,"* Lynmarie Thompson

**Fumitoshi Kato**, *"Synthesis of Transition Metal Ion Doped Metal Benzenechalcogenolate Clusters,"* Kevin R. Kittilstved

**Piyachai Khomein**, *"Amphiphilic Assemblies with Responsive Characteristics at Surfaces and Interfaces,"* S. Thayumanavan

**Ryan F. Landis**, *"Hybridized Polymeric Nano-assemblies: Key Insights into Addressing MDR Infections,"* Vincent M. Rotello

**Bin Liu**, *"Molecular Designs of Novel Responsive Assemblies for Therapeutic Delivery Applications,"* S. Thayumanavan

**Xiaorong Liu**, *"Multiscale Simulations of Intrinsically Disordered Proteins,"* Jianhan Chen

**Derek J. MacPherson**, *"Probing Apoptotic Caspase Allostery and Exosite Interactions for Alternative Regulation,"* Jeanne A. Hardy

**Mahalia (Mac) Serrano**, *"Enhanced Mass Spectrometric Analysis of Peptides and Proteins Using Polymeric Reverse Micelles,"* Richard W. Vachet

**Uma Sridhar**, *"Design and Self-Assembly of Responsive Scaffolds for Food and Sensing Applications,"* S. Thayumanavan

**Qinfang Sun**, *"Simulating Hydrogen Bonded Clusters and Zeolite Clusters for Renewable Energy Applications,"* Scott Auerbach

**Prabhat Tripathi**, *"Voltage-Driven Polyelectrolyte Complexation Inside a Nanopore,"* Murugappan Muthukumar (PSE)

**Li-Sheng (Cola) Wang**, *"Development of Functional Biomaterials Using Protein Building Blocks,"* Vincent M. Rotello

**Bib Yang**, *"Engineering Outer Membrane Protein G (OmpG) for the Detection of Human Carbonic Anhydrases,"* Min Chen

**Bo Zhao**, *"Protein Detection and Structural Characterization by Mass Spectrometry Using Supramolecular Assemblies and Small Molecules,"* S. Thayumanavan & Richard Vachet



# iCons by Scott Auerbach, iCons Director

The 9th year of the UMass iCons Program brought new excitement, accomplishments, and opportunities to this signature program that bridges all undergraduate majors of science and engineering.

This year we welcomed the 9th cohort to iCons – the so-called “9th Bit” – a name that recognizes the massive impact of information science on problem-solving in the 21st century. This brings the total number of students who’ve entered iCons to about 500. Our current students continue to see their problem-solving ideas grow legs. iCons students **Meg Davis** and **Radha Dave** were awarded the Sustainability Innovation & Engagement Award for 2019 for their proposal “Water Metering in Showers.” This idea was hatched during the iCons 1 student-team-created case study at the end of their 1st year. Now that they have funding, we are excited to see how their research yields reduced water and energy usage on campus. We’re also proud of our 10 iCons students who are Chleck Scholars – each supported by a \$10,000 annual scholarship to help pay for college, generously funded by the Chleck Foundation.

Our alumni community continues to grow – having graduated our 6th cohort this May, there are now about 180 graduates of the program. We were so pleased when 3rd Axis alum **Samantha Giffen** returned to campus on May 2nd to receive the second annual Mahoney iCons Alumni Award. Samantha, who is pursuing a PhD in public health at Harvard, received this award for her demonstration of the iCons approach in the workplace and for her continued efforts to support the iCons Program. Our other graduates continue to do great things and get recognized for working on innovative solutions to big problems, such as iCons 1st Class alum Isaac Han of the Wyss Institute for Biologically Inspired Engineering at Harvard; and iCons 3rd Axis alum **Katharine Greco**, who is pursuing her PhD in chemical engineering at MIT, and who won the award for best video abstract at the MIT International Conference of Applied Energy in May 2019.

The iCons 1 instructional team benefited this spring from the expertise of our newest faculty member, Biology Dept. professor **Christiane Healey**, the first recipient of the Mahoney iCons Teaching Award. The gift behind this award was generously given to help the iCons Program diversify its instructional team. Prof. Healey’s expertise as a biologist was particularly helpful as students studied amphibious decline in the second case study of the iCons 1 course in Spring 2019. Students learned to create models, isolating the relative effects of various human and natural causes on amphibious population decline. We welcome Prof. Healey to the iCons Program!

We’re delighted to announce the exciting news that, thanks to the generous support of the Mahoney Family, the iCons Program has been given the green-light to begin work on launching a new track in the problem area of Food and Water. This adds to the existing problem tracks in Biomedicine/Biosystems (health of people // health of the planet), and Renewable Energy (sustainably powering the planet). Launching an iCons Food/Water track involves increasing the number of students accepted into iCons by 50%, to 90 students per year, expands the impact of iCons across campus to new student and faculty populations, and most important, further prepares our students to be leaders in science and technology with the attitudes, knowledge, and skills needed to solve the inherently multi-faceted problems facing society.

We thank all those who have helped the UMass iCons Program have another banner year, especially our corporate sponsors – Anika Therapeutics (Bedford, MA), Waters Corporation (Milford, MA), and Zipher Medical Affairs (Marion, MA). We also gratefully acknowledge generous support from our philanthropic donors, especially the Mahoney Family and the Chleck Foundation.



The 6th graduating class of the UMass iCons Program – the so-called 6th Sense – celebrating together with iCons Director and Chemistry Professor Justin Fermann



Dominique Carey (right) with research advisor, Prof. Lynmarie Thompson

Dominique Carey, Chemistry BS '19, was a recipient of the iCons Crowley-Nowick Leadership award that recognizes students who embody the iCons mission of open-mindedness, strong leadership, and teamwork.

As part of the program, during the summer after her freshman year, Carey worked as an educational innovation intern. Her work focused on developing iCons-inspired case studies for high school students. iCons has helped her feel empowered by science. “We were thinking of making mechanical krill to solve the great pacific garbage patch for our first iCons project,” she recalls, “and of course it distilled way down from that, but it was kind of cool to be able to be like ‘yeah, let’s do anything!’” Carey also had a hand in networking within the iCons student body and encouraged the iCons Alumni Network (iCan) members to work with students on resumes and career advancement.

# Seminar

by Mingxu You, Seminar Chair

The 2018-19 UMass Amherst Department of Chemistry seminar series brought many outstanding scientists to the campus to share their insights and recent discoveries. These speakers included several distinguished members representing the diverse field of chemistry.

In September, **Professor Paula T. Hammond** from MIT presented the **Stein-Covestro Honorary Seminar in Polymer Chemistry**. Prof. Hammond was elected into the National Academy of Engineering, the National Academy of Medicine, and the American Academy of Arts and Sciences. As an internationally recognized leader in polymer chemistry, she has developed novel responsive polymer architectures for targeted drug and gene delivery, and has engineered self-assembled materials systems for electrochemical energy devices. Her seminar focused on the construction and application of polyelectrolytes for drug delivery.

**Professor Jack W. Szostak** from Harvard Medical School and Harvard University presented the **William E. Mahoney Annual Lecture** in October. He is a member of the National Academy of Sciences and the American Academy of Arts and Sciences. Prof. Szostak's research on telomere structure and function was recognized by the 2009 Nobel Prize in Physiology or Medicine. In addition, he has developed an approach to in vitro select functional RNA and DNA aptamers from large pools of random sequences. During this lecture, he discussed his recent research efforts in the laboratory synthesis of self-replicating systems and the origins of life.

**Professor John F. Hartwig** from the University of California Berkeley was the **Marvin D. Rausch Lecturer in Organometallic Chemistry** this year. Prof. Hartwig is a distinguished scientist in the fields of catalysis and organic chemistry. He has developed several transition metal-catalyzed new reactions including a selective functionalization of alkanes and formation of important carbon-carbon and carbon-heteroatom linkages. He is also a member of the National Academy of Sciences and the American Academy of Arts and Sciences. Prof. Hartwig has been honored with numerous awards including a 2019 Wolf Prize in Chemistry. In this seminar, he talked about some recent discoveries in selective catalytic functionalization of C-H bonds.

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**. In spring 2019, we welcomed **Professor Clare P. Grey** from Cambridge University as the 5-College Lecturer. Prof. Grey is a Fellow of the Royal Society and a foreign member of the American Academy of Arts and Sciences. She has received an array of awards and honorary lectureships including the Gunther Laukien Prize and Davy Medal. Her presentation at UMass was about the use of solid state NMR and diffraction-based approaches to develop and optimize the energy storage, conversion, and carbon capture of Li-ion and other types of batteries and fuel cells.

In addition to these 'named' seminar speakers, the department had many luminaries within the field of chemistry participate in our seminar program in 2018-19, including **Prof. Christopher N. Bowman** (U. Colorado Boulder), **Dr. Chris Mundy** (Pacific Northwest National Lab), **Prof. Eva Nogales** (UC Berkeley), **Prof. Frantisek Turecek** (U. Washington), **Prof. Matthew B. Francis** (UC Berkeley), **Prof. Marc A. Hillmyer** (U. Minnesota), **Prof. Yi Lu** (U. Illinois), **Prof. Wei Yang** (Florida State U.), **Prof. Ke Zhang** (Northeastern U.), **Prof. Javier Vela** (Iowa State U.), **Prof. Michael Cohen** (Oregon Health & Science U.), **Prof. J. D. Tovar** (Johns Hopkins U.), **Prof. Debbie Crans** (Colorado State U.), **Dr. Reshma Shetty** (Ginkgo Bioworks), **Prof. John E. Straub** (Boston U.), **Prof. Haipeng Liu** (Wayne State U.), **Prof. Charles R. Sanders** (Vanderbilt U.), **Prof. Daniel T. Chiu** (U. Washington), **Prof. Robert S. Langer** (MIT), **Prof. Paul J. Hergenrother** (U. Illinois), **Prof. Amanda Hargrove** (Duke U.), **Prof. Kwok-Fan Chow** (UMass Lowell), and **Prof. Abraham Badu-Tawiah** (Ohio State U.). 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 <https://www.umass.edu/chemistry/events-seminars>. We look forward to another exciting seminar series next year!



Professors Paula T. Hammond, Richard Stein, and Don Wardius (Covestro)



Professor Jack Szostak and Robert Mahoney



Professors Richard Vachet, Jane Rausch, and John Hartwig



Professors Clare Grey and Scott Auerbach



# Outreach

## Girls Inc. EUREKA!

**Dr. Lara Al-Hariri**, UMass Chemistry, developed the workshop “Explore Fun Chemical Reactions: Making Soap” to encourage girls in the Eureka! program to be excited about chemistry. Dr. Al-Hariri, in collaboration with **Dr. Mingxu You** and **Dr. Ruthanne Paradise**, has been offering this workshop for the last three summers. Eureka! is an outreach program at UMass Amherst in partnership with Girls Inc. of Holyoke. The program aims to address the gender gap in the field of STEM through motivating and empowering girls through a hands-on series of workshops. It is crucial for the girls to see women in science leading these workshops, and be a role model for them.

The workshop is designed to teach the girls skills and chemical concepts by making soap. They perform an organic chemistry reaction (the hydrolysis of an ester) that keeps them engaged by preparing an item they use daily (soap). During the workshop, the girls learn about the pH scale, the appropriate range of pH for soap, the soap foam level, and its relationship to the hardness of water — the basics of how soap works.



The sixteen Eureka Scholars “Rookies,” rising 8th-grade girls, used the analytical laboratory in ISB and their first check was with Dr. Paradise to ensure they were wearing proper

safety attire. Dr. Al-Hariri gave them a short overview of the experiment, explaining how they would convert coconut oil into soap through a chemical reaction called saponification. She showed them a prepared sample of a soap bar and discussed how they could customize their soap by choosing the fragrances, colorant, and mold shape. Their faces bloomed with excitement. The girls were then provided with a detailed procedure and the three instructors began to guide them through the process.

Twenty minutes into the workshop, the girls added the concentrated sodium hydroxide to the coconut oil and the reaction began. While waiting for the reaction to complete, Dr. You introduced them to the pH scale and showed them the pH of items they are familiar with (milk, drain cleaner, and battery acid) through a simulation. They put that knowledge into practice at the end of the workshop to decide if their soap is usable. They also learned about how

soap works through an activity in which they use a rope (carbon long chain/hydrophobic) and balloon (COO-/hydrophilic) as models of a soap molecule to form a micelle. The

girls learned and understood the hydrophobic and hydrophilic parts of the soap and their contribution to how soap works.



Dr. Al-Hariri says, “It is amazing when they ask with excitement when they will be able to retrieve their soap bars and take pictures to let their friends on social media know that they made soap.”

This summer, the workshop will be offered as a two-day workshop to provide the girls more time to enjoy all the activities.

Dr. Al-Hariri says, “Eureka gives me a unique opportunity to be in contact with this age group and help them get excited about science. I want girls to know that science is the field for them through this hands-on, fun science experiment.”



## Grant Helping Andrew Increase Research Opportunities for Community College Students



Prof. Trisha Andrew and Emerson Alexander

Trisha L. Andrew, associate professor of chemistry, received a \$2,500 L'Oréal USA Changing the Face of STEM grant to increase hands-on research opportunities for community college students.

During the 2018-19 academic year, Andrew and her research group trained interns from Springfield Technical Community College (STCC) to create garment-integrated sensors, an effort that she hopes will “entice a diverse student population to become scientists and fortify the number of underrepresented students in chemistry and engineering.”

Andrew Outreach continued

STCC offers students a program called STEM Starter Academy to enhance students' readiness for STEM jobs or to transfer to a four-year academic STEM program. Andrew has previously participated in annual "maker" events organized by STCC and has worked with STCC faculty to encourage graduates of its Starter Academy to pursue degrees at UMass Amherst.

For example, Emerson Alexander, a recent graduate of the STEM Starter Academy, worked in Andrew's lab to develop fabric patches that turn bright pink when the wearer has been exposed to a damaging level of ultraviolet light. Emerson, who is currently enrolled in the pre-dental major at STCC, graduated from Minnechaug Regional High School in 2018 with several honors including a John and Abigail Adams Scholarship.

## Physical Sciences Building Ribbon Cutting

The Physical Sciences Building (PSB) ribbon cutting ceremony on April 4, 2019, included speeches by Governor Charlie Baker, State Senator Jo Comerford, State Representative Mindy Domb, as well as UMass system President Martin Meehan, Trustee Mary Burns, UMass Amherst Chancellor Kumble Subbaswamy, CNS Dean Tricia Serio, Associate Dean Mark Tuominen, and **Chemistry Head Richard Vachet**.

"We were pleased to invest in the new Physical Sciences Building, which will serve as a hub for the natural sciences at UMass Amherst," Baker said. "The facility's expansion will help foster new research and career opportunities, which will help support the STEM workforce pipeline here in Massachusetts."

"This project reflects the significance of the Commonwealth's investment in faculty excellence, scientific discovery and student success at UMass Amherst," said UMass President Marty Meehan.

"And it strengthens UMass Amherst's position as a top-tier public research university that prepares students to thrive in the high-demand STEM fields that are so important to the future of Massachusetts."

During laboratory tours with UMass President Marty Meehan, Chancellor Subbaswamy, and Trustee Mary Burns, **Professor S. Thayumanavan** explained his research on developing nanoparticles for delivering therapeutic molecules and proteins for cancer, and **Professor Trisha Andrew** talked about her smart garments for activity and movement. Other chemistry research groups with specialized laboratories in the PSB are headed by **Professor Michael Barnes**, **Professor Kevin Kittilstved**, **Professor D. Venkataraman**, and incoming faculty **Professor James Walsh** and **Professor Joseph DuChene** (joining the department in January).

Chancellor Kumble Subbaswamy said, "This complex is home to the very best facilities in physics and chemistry, enhancing the research capability for our faculty and students in the College of Natural Sciences and providing the STEM talent that is essential for the state's innovation economy. We're deeply grateful for the governor's support and the state's investment in UMass Amherst." The Chancellor presented Gov. Baker with a hockey stick signed by the UMass Hockey Team (shown top left) to celebrate the team's historic season that brought them to the Frozen Four finals.





# 2019 Undergraduate Awards

The annual Senior and Awards Dinner was held on Friday, April 26th in the Marriott Room at the Campus Center. Over a hundred students, parents, faculty, and staff joined to recognize the hard work and dedication of our 26 graduating seniors and to honor our students who have proven themselves to be among the very best this University 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.



Prof. Michael Knapp, Obinnaya Okereke, and Prof. Scott Auerbach

## Academic Awards

### American Chemical Society (ACS) Hach Scholarships

Olivia Pietrobuono and George Ryan

### ACS Undergraduate Award in Analytical Chemistry

Ryan Thai

### CRC Press Chemistry Achievement Award

Laura Casey, Ethan Goulart, and Obinnaya Okereke

### Edward Shapiro Fund

Allison Burke, Nicholas Heller, Samuel Knight,

Mark Leon-Duque, and Ryan Pham

### George R. Richason, Jr. Scholarship

Bryanna Lexus Freitas

### Jay A. Pirog Scholarship

Eliadine Desir

### John A. Chandler Memorial Scholarship

Yankai (Mark) Xiang

### Robert Maxwell Williams Memorial Scholarship

Jacob Carroll, Sinclair Emans, and Jennifer Marino

### Royal Society of Chemistry Certificate of Excellence

Ryan Thai

### Thomas R. "Casey" Stengle Scholarship

Olivia Pietrobuono

## Research Awards

### ACS Undergraduate Award in Inorganic Chemistry

Ruby Nelson

### ACS Undergraduate Award in Organic Chemistry

Francisca Perez

### ACS Undergraduate Award in Physical Chemistry

Tristan Heck



Tristan Heck

### Chemistry Undergraduate Research Fund

Samuel Stroup

### Dr. Uche Anyanwu Memorial Fund

Gisele Andree, Benjamin Avramidis, Tiernan Kennedy

### J.F.B. Fund for Undergraduate Research

Taylor Garrey

### Mr. Tompkins Award

Cameron Kaminsky and Mark Leon-Duque

### Oliver Zajicek Memorial Scholarship Award

Sara Chedid

### Professor Jack Ragle Endowed Fund in Chemistry

Tristan Heck

### Roger G. Bates Chemistry Fund

Gillian Willcox

### Sir Harold W. Kroto and Steve F.A.

### Acquah GEOSSET Award

Dominique Carey

### Tarselli Family Research Award

Tiernan Kennedy, Jason Biundo



Gillian Willcox and Prof. Lila Gierasch

## Departmental Awards

### ACS-Connecticut Valley Section Student Award

Mark Leon-Duque

### American Chemical Society Membership Awards

Luke He and Tiernan Kennedy

### American Institute of Chemists Award

Gisele Andree

### Departmental Recognition Award

Gisele Andree and

Sara Chedid

### Distinguished Undergraduate

### Instructor Award in Honor of

### Earl J. McWhorter and George R. Richason, Jr.

Lara Al-Hariri

### Distinguished Graduate Teaching Assistant Award in Honor of George R. Richason, Jr.

Yanfeng Li

### Distinguished Undergraduate Teaching Assistant Award in Honor of George R. Richason, Jr.

Luke He

### Positron Award

Gisele Andree

### Richard W. Fessenden Award

Gisele Andree

### Senior Class Award

Gisele Andree



Prof. Ruthanne Paradise, Gisele Andree, and Prof. Min Chen





## Chemistry Seniors 2019

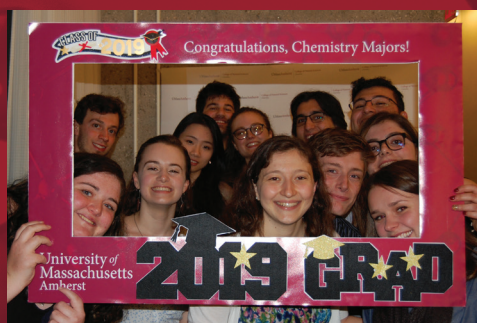
Gisele Andree\*  
Jean Arnaud\*  
Benjamin Avramidis  
Allison Burke\*  
Dominique Carey  
Sara Chedid\*  
Christopher Chinman\*  
Alexander Demokritou\*  
Bianca Edozie  
Nicolas Gupta  
Jessica Jones  
Kyle Koczera\*  
Mark Leon-Duque\*  
Zhaoxia Li  
Madison Montagna  
Amber Nehring\*

Julie Novelli\*  
Francisca Perez  
Alexandra Sahagian  
Alexander Santoro\*  
Dana Sebestyen\*

Fall 2019  
Minji Kim  
Xavier Sanchez-Felix  
Andreos Valle

BS with Concentration  
in Chemistry  
Tushar Bahl  
Richard Maxson

\* American Chemical Society certification





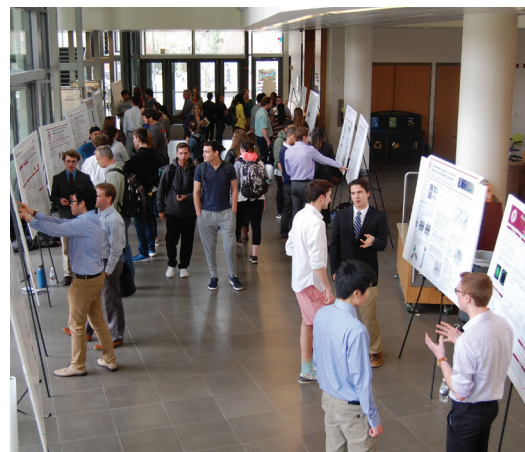
# undergraduate Research Projects

## Undergraduate Poster Award Winners

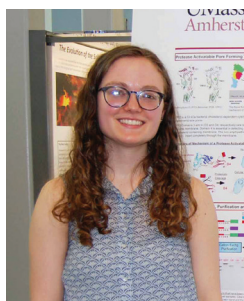
The Dr. Uche Anyanwu Memorial Fund recognizes the top three research posters presented by chemistry majors, and was established by Dr. Ucheoma O. Akobundu to honor her late husband.

Dr. Uche Anyanwu, the first member of the D. Venkataraman (DV) group, was awarded his PhD in 2005 for his work on “Soluble Polymer-supported Catalysts and Initiators.” Anyanwu developed polymer-supported chiral organic ligands for transition metal asymmetric catalysis to address the major issue of recyclability in conventional homogeneous catalysis. He also developed cleavable diblock copolymers for fabrication of nanoporous thin films. After his Ph.D, Uche joined Momentive as a Senior Scientist. Anyanwu is remembered for being an excellent scientist, artist, sportsman, and a kind human being.

Of the sixteen posters presented in the ISB atrium this year, the three award recipients were Gisele Andree, Benjamin Avamidis, and Tiernan Kennedy.



### Development of a Protease Activatable Pore-Forming Toxin by Gisele Andree



Cancer is an incredibly difficult disease to treat as it will often evolve and advance beyond the initial treatment methods; thus, finding new ways to eradicate cancer cells is tremendously important. The development of protease activatable pore forming toxins that target cancer cells is one way to tackle this problem. Using the cytolysin, perfringolysin O (PFO), large proteins are attached to the C-terminus of PFO thus inhibiting its normal cytotoxic activity. These inhibitor proteins are attached via an amino acid linker that contains a cleavage sequence of a specific protease. Once in the presence of this protease, the inhibitor proteins are cleaved off and PFO can regain its cytotoxic ability. Constructs can be designed to only be activated by proteases that are over-expressed and secreted from cancer cells, so these proteins would only be toxic towards these types of cells. My studies with Prof. Min Chen aim to develop a PFO-fusion

protein that can be cytotoxically activated through proteolysis by matrix metalloprotease-2 (MMP-2), a protease overexpressed and secreted in many types of cancers. Different protease-activatable PFO-fusion proteins were designed using green fluorescent protein (GFP) and maltose binding protein (MBP) as the inhibitor proteins and the cytotoxic activities of cleaved and un-cleaved constructs are tested via hemolytic assays.

### Using a Cluster Method to Computationally Describe Adsorption Processes in HZSM-5 Zeolite

by Benjamin Avramidis



Zeolites are solid, nanoporous crystal-structured aluminosilicate catalysts that are used widely in industry as aids in processing and separating fuel from crude oil. Given our society's insatiable hunger for energy as well as the restrictions and faults associated with the burning of fossil fuels, our lab focuses on the possible contributions zeolites may have in synthesizing reusable green biofuels. To investigate this possibility, we use computers to aid in the heavy quantum computations required to model interactions occurring within zeolite pores which eventually produce biofuel precursors. A question concerning computational chemists when faced with modeling a large system like zeolite is, "How many atoms do we include in our model?" My role as a researcher in Prof. Scott M. Auerbach's group has been to ask that same question in regard to single molecule adsorption within HZSM-5 zeolite. The adsorption process, taken to be the energy

associated for a molecule to sit comfortably within a pore, is arguably the most important step in all zeolite catalysis. Utilizing a previously developed cluster method, the atoms required to properly describe adsorption are determined to be the adsorbate molecule and the few essential atoms involved at the zeolite active site. By having each atom emit a sphere of radius  $\delta$  chosen by the user, the surrounding atoms of zeolite which fall within collective spheres determine which atoms represent the model. The importance of this method lies within the idea that by systematically increasing  $\delta$ , we eventually reach a point where energy change is independent of  $\delta$ , therefore obtaining the least number of atoms required to describe our system. Our hope is that this delta cluster method will make computation of adsorption processes easier, saving time and computational resources.

## DNA-Mediated Assembly of Bacterial Chemoreceptor Complexes by Tiernan Kennedy



Our research in the Thompson Lab focuses on uncovering the signal propagation mechanism in bacterial chemotaxis receptors. This highly conserved class of transmembrane proteins binds attractant and repellent ligands and in turn controls the activity of the bacterial flagellar motor, but the physical mechanism for the process is poorly understood. However, our research is complicated by the fact the chemoreceptors form highly complicated signaling arrays that are difficult to replicate and control in vitro.

Over the past year and a half, I have worked toward developing a novel in vivo assembly of these receptor complexes using a DNA origami scaffold. We believe that attaching our protein complexes to the base of a DNA tetrahedron will provide the control over receptor geometry needed to test some of our most critical hypothesis. To date I have optimized a key DNA modification reaction needed to attach the tetrahedron to our protein and have shown that the necessary DNA origami scaffold can be synthesized. We hope that when this assembly method is completed it will provide the control needed to gain a much deeper understanding of our protein. Figure 1 shows our proposed assembly constructs. Attaching protein dimers to the vertices of a DNA tetrahedron (top) provides native-like trimers-of-dimers of chemoreceptors. Each protein dimer is depicted in gray with accessory proteins for complex formation in blue and teal.

## Rising Researcher Awards

### Chemistry Undergraduates Bianca Edozie and Mark Leon-Duque Honored as Rising Researchers

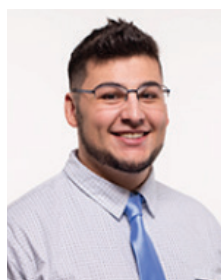


Eight students from across campus were honored with the Rising Researcher Awards in recognition of their demonstrated leadership and impact in their chosen field of study. Commonwealth Honors College student Bianca Edozie '19, a double major in chemistry, and biochemistry and molecular biology, works on projects that explore

various behavioral aspects of microtubules—stiff, structural elements found in animal cells. Microtubules help form the spindle apparatus during cell division and can act as an intra-cellular transport system, among other things.

Her current project centers on creating “tactoids”, biologically relevant microtubule organizations that act as model mitotic spindles in the lab. The model allows Edozie and other researchers to explore the effects of proteins and enzymes on mitotic spindle organization. She recently published a paper with Jennifer Ross (physics) in the journal *Soft Matter*. “Bianca is a brilliant student and one of the hardest working people I have ever met,” says Ross. Ross notes that Edozie represented UMass at a Research Experience for Undergraduates, which took place at Brandeis University. “She took new data, and performed incredibly difficult dynamics experiments that will continue this year as part of her honors thesis. This work will likely result in a second manuscript. I see no end to her possible future leadership in whatever field she continues,” says Ross.

“My project has been more than just the research itself, but more specifically, what the research required me to learn as an aspiring scientist. I’ve acquired a wealth of knowledge, both new and supplemental to my education in the classroom,” says Edozie.



In recognition of his demonstrated leadership, Mark Leon-Duque '19, was honored with the Rising Researcher Award. A sophomore seminar class introduced Leon-Duque to research projects underway on campus. “I promptly contacted Dr. Mingxu You (chemistry) asking to shadow his lab members and by the spring semester, I was working on a project, handling the experimental portions and some of the analysis,” says Leon-Duque.

In the first two years of his time in the You lab, Leon-Duque worked closely with research fellow Aruni P.K.K. Karunanayake Mudiyanseleg. Together they developed a new RNA-based imaging system for detecting small RNA molecules within live cells. “Our efforts and the resulting manuscript was published in *The Journal of The American Chemical Society*. I tested a few of our designs independently that earned me my name as third co-author on the publication. Currently, I am working independently on expanding this imaging system to apply to other small molecules,” says Leon-Duque.

As for the future, Leon-Duque says, “Publishing my first paper with Aruni and all the other contributors gave me such an exhilarated rush, a true sense of accomplishment. The project also taught me things that are completely out of the scope of the typical chemistry undergrad curriculum. I know that I want to do research, whether it will be in academia or in industry remains to be revealed. Nevertheless, I feel my sense of purpose and I will tread this path with diligence and my best effort,” Leon-Duque’s principal investigator, Mingxu You, adds: “Mark has demonstrated great potential to be an independent scientist. He can learn new techniques and knowledge very quickly and his results are repeatable and trustable.”



## Chemistry Clubs

The **UMass Chemistry Club** is dedicated to increasing interest in chemistry and getting people excited about it. In the spring, the club hosted events in the form of an ice cream social and participated in the club expo as well as parents' weekend. At the club expo, we were able to recruit new members from a variety of majors from Biochemistry to English. In order to meet all of the club members, new and old, we also hosted an ice cream social where we made Dippin' Dots by using liquid nitrogen and a variety of ice cream flavors. During parents' weekend, we held chemical demonstrations for families which ranged from elephant toothpaste to ferrofluid. In the future, we hope to increase club member interaction by holding a movie night and also a holiday themed event in the fall.

The **ACS Club at UMass** is a student chapter and a wonderful community resource for chemistry majors. Meetings focus on either career/grad school prep, research presentations from faculty, or cool hands-on chemistry activities. The club is an inclusive space dedicated to helping chemistry majors network, learn, prepare, and have fun!

## CURE-REU Program Summer 2019 by Ruthanne Paradise

Each summer, the Chemistry department hosts undergraduate students for a research experience that runs for ten weeks. This year sixteen students and four different REU programs were involved in the educational programming. This experience was funded by Collaborative Undergraduate Research in Energy-Research Experience for Undergraduates (CURE-REU) NSF grant, the Center for Autonomous Chemistry (CAC), Roger Bates Chemistry Fund, and Kevin Kittilstved's Career REU. Prof. Paradise directs the educational portion of the program.

This summer, REU students met twice a week. On Tuesdays, participants met with scholars from the LSAMP and Lee-SIPP program and worked on professional development and designing their final poster. On Thursdays, we worked on designing an educational outreach lesson as well as writing a journal article to share research results.

This summer was a great success; students learned more about what kind of research they enjoyed. The final poster presentation was also a success; students collaborated on educational videos on topics ranging from puppets to animation to posters.



2019 CURE-REU participants



CNS Dean Tricia Serio, Sam, and Prof. Scott Auerbach



Dean Serio and Sam the Minuteman

## Pi(e) a Professor

CNS sponsored an Ice Cream Social for the college that included a Pi(e) a Professor booth to raise money for the CNS Student Emergency Fund. A few chemistry faculty including Scott Auerbach, Christopher McDaniel, Hans Mentzen, and Thomas Whelan volunteered, and each pie tossed earned a dollar donation for the cause. CNS Dean Tricia Serio also took a few pies in good fun, and Sam the Minuteman was on hand to cheer on the crowd and toss a few pies.



Prof. Thomas Whelan



Ben Avramidis (Chemistry '19) pieing Prof. Scott Auerbach



Zhaoxia Li (Chemistry '19) and Sara Chedid (Chemistry '19)

## Staff Notes

We welcomed **Brian Lochner** as our new Bookkeeping Assistant/Procard Records Manager. He prepares accounting reports and processes recharges, purchase orders, travel forms and invoices. He plans to take classes part-time in Fall 2019 to finish his Bachelor's Degree in Applied Mathematics.

**Laura Sedberry** joined us last fall as the new Seminar/Safety/Alumni Coordinator. She obtained a BS in Business Management and a Master's in Social Work from Indiana University-Purdue University Indianapolis. She has previously worked as a therapist to children and families and for non-profit organizations. Laura is excited to be a part of the Chemistry Department and loves the energy of being in an academic setting.

**Tania Wellen** has changed roles in chemistry and is now our Personnel Coordinator. She prepares staff and postdoc appointments, orients visiting scholars, makes sure everyone is paid in a timely manner, and much more.

**Sovann-Malis Loeung** is the new administrative assistant for both the Chemistry-Biology Interface (CBI) and UMass Biotech Training (BTP) programs. Previously, she was an Administrative Assistant in the College of Education and earned a Bachelor's degree in Social Justice Studies from University Without Walls in 2017.

### Vicki Hubby Wins CNS Outstanding Staff Award

Chemistry's Business Manager Vicki Hubby has won a CNS Outstanding Staff Award. This award recognizes the crucial role played by staff members in facilitating the success of the College of Natural Sciences.



Vicki is responsible for managing the department's instructional and general operating budget. The new glassware for the organic labs, those amazing new instruments in the upper level labs, events honoring our wonderful students, graduate student fellowships—she figures out how to pay for all of it! Vicki also sets up laboratory startup funds for new faculty and helps faculty manage budgets from external and internal grants. If it's related to purchasing, budgets, and balances, Vicki knows how to do it. Her responsibilities are very significant undertakings, given that our student enrollments and faculty research funding has more than doubled in the last 10 years. The scale of the operation in the Chemistry Department has increased dramatically since Vicki arrived in 1999, and she has met the challenges with incredible ability, creativity, and grace.



jms with Lila Gierasch

### Graduate Program Coordinator, jms, Retires

by D. Venkataraman (GPD) and Mahdieh Yazdani (Graduate Student)

This May, JM Stowe (jms) formally retired as Graduate Program Coordinator. She joined the Chemistry Department in 1996, when she was hired by Department Head Lila Gierasch to be the Head's Assistant. jms transitioned to Graduate Program Coordinator in 2005 because she wanted to work with students again—prior to her time in chemistry, she was the Graduate Program Coordinator in the Art Department. Among many other duties, jms ensured that the Chemistry graduate program of >125 students ran smoothly. Her unique and cheerful emails were many graduate students' first introduction to the department. She kept track of every graduate student's progress, advised them regarding degree requirements, graduate school paperwork and deadlines, and other aspects of

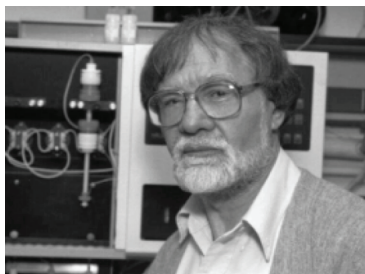
their graduate life. She cared deeply about students' personal well-being as well as their academic progress. Students note that jms was always welcoming and available to answer their questions. They fondly remember jms as akin to a caring parent who would listen to their personal struggles, offer support, and follow up to ensure that their problems were resolved. We thank her, and wish her a very happy retired life!



# In Memoriam

## Louis Carpino, Quintessential Organic Chemist

by Peter Lillya



Early this year, we lost one of the foundation blocks upon which today's Department and this modern research university were built. In 1954, with a PhD from the University of Illinois and a post-doctoral year at the University of South

Carolina, Louis Carpino joined the UMass chemistry faculty. By 1956, a paper from his laboratory was published in *Chemistry & Industry*, one of 14 early single-author publications. Although UMass had granted PhD degrees in chemistry since 1915, the arrival of John Brandts, Lou Carpino and Dick Stein in the 1950s gave the Department cutting-edge research the current Department was built upon.

Lou's work, which he described in a 1973 *Accounts of Chemical Research* paper, ranged widely. But he is best known and honored for the versatile amino protecting groups he created, the acid-sensitive *t*-Boc and base-sensitive Fmoc groups. These are still the premier amino protecting groups in organic synthesis, and the Fmoc group became an essential feature of automated peptide synthesis using the Merrifield "solid state" method. He was honored with the 1992 Hirshmann Award in Peptide Chemistry.

Louis was notable for his embrace of venturesome sabbatical leaves at institutions like Mainz University in Germany, the University of Padova in Italy, Orsay in France and the Institute of Organic Chemistry in Lodz, Poland. A planned year in Iran was thwarted by the Iranian revolution while the Carpino family was in transit to Iran.

In addition to his research achievements, Lou was an outstanding teacher of organic chemistry. This writer audited his graduate course in organic synthesis that was full of the latest developments and Lou's personal insights which kept me returning lecture after lecture. His organic cumulative exams were famous for the challenges his "roadmap" questions posed including one that was partly in German! (Organic chemists read the German literature in those days.) It was a loss for the Department's teaching program but a gain for peptide chemistry when Lou converted to a research appointment to focus on peptide synthesis.

Lou was prized by his colleagues as a willing contributor to our common enterprise. His knowledge of organic chemistry spread far beyond his specific research interests and he was the first person many of his close colleagues would consult about issues that arose in the course of their research. Even in his retirement he remained an active researcher and a valued

chemical consultant for his younger colleagues, spending most of the day at his office, walking home for lunch, then returning in the afternoon. Lou's characteristic modesty would make him uncomfortable with even the smallest degree of recognition. But his contributions to organic chemistry and to our UMass chemical community compel us to celebrate him as a great and well-loved colleague.

## Paul Drummond by Peter Lillya



When Paul Drummond died unexpectedly in December of 2018, it reminded me how important he had been to the creation of what we are today. It has been attributed to Napoleon, a keen appreciator of the importance of logistics, that "an army marches on its stomach." Louis Quin, who became Head in 1986, realized that a chemistry department

requires laboratories that function effectively, so that faculty, students, and staff can succeed in their endeavors. He conceived the position of "operations manager" and called his friend at the FMC Corp., Paul Drummond. Paul had enjoyed a successful industrial career beginning as an organic chemist and finishing by leading FMC's Research and Development Department. How fortunate we are that Paul answered Louis's call. Paul arrived in Amherst, rolled up his sleeves, and went to work, helping to set the department on the upward course we have navigated since.

Prior to that time, the functions of an operations manager were undertaken by faculty as a part-time job, with limited success. Paul recognized instantly that the university Physical Plant had to be enlisted as part of a team to maintain and improve our laboratories. This required change that didn't come easily. Paul established his credibility by making our needs clear and pursuing them unrelentingly until they were met. Paul acquired a reputation as someone who always meant what he said and whose word could be trusted. Late completion, previously the custom, became rarer as time passed and a cooperative relationship developed. The Department's research and teaching programs were beneficiaries. Paul was recognized with the Chancellor's Award for outstanding service.

Those who benefitted most were the new faculty who were such a vital part of renewal and who spearheaded the new initiative to form a group within Chemistry committed to tackling biological questions with the tools of chemistry. New researchers needed working laboratories and equipment ready when they arrived, not 6-8 months later. Paul made it a priority to make this happen. He was an essential part of our Department's—as well as the University's—progress and development.

# Alumni

## We are a UMass Family by Diane Stengle '72, '80 PhD

My career path has been varied, and includes experience outside of chemistry. My education began at a small local Catholic college, and then led to UMass (BS, 1972). I was looking for more challenges in applied and theoretical aspects of chemistry. UMass provided the environment, both materially and intellectually, for me to explore many options, including teaching (as a TA). The closeness of the chemistry department was important for me, and this is still the case today. I remember students felt as if we were members of a community of scientists, including faculty (and my future husband!). I sense that same spirit today, as I come back to the UMass chemistry department to spend time and share with the current community.



Diane Stengle (right) with daughter Anne Stengle

Casey, particularly, had a love for the history of the chemistry department. I still have his copy of a biography of Charles Goessmann. It is another way to experience community, to be part of the tradition upon which the department was built and continues. After earning my Chemistry PhD in 1980 from UMass, I went into industry for the challenge of applied research, which I learned at UMass from the dedicated faculty and graduate students. After several years at Monsanto in Springfield, I took a few years off and got an MA in Religious Studies from another local Catholic college. When Casey died, in 1993, I returned to chemistry, this time as a faculty member at Holyoke Community College (HCC). I remembered how much I had enjoyed my work as a TA, and wanted to have another experience of sharing my interest in chemistry with students. I have been teaching at HCC ever since.



Thomas R. "Casey" Stengle and John Babiec (PhD '66)

UMass provided me with skills and perspective besides the educational (knowledge) background. It also showed me the value and importance of the community of scientists as we do our work. That closeness of purpose and activity is essential, and it applies as much to my teaching now, as it did for me as a student in 1972. Anne (our daughter) chose biology as her field (BS, 2010 and PhD in Organismic and Developmental Biology, 2018, both from UMass) but is now also teaching chemistry at HCC. She could not get away from chemistry, with two parents having a love for it! I believe that our family is a reflection and an extension of the community of the chemistry department at UMass. We are a UMass family!

### Thomas R. "Casey" Stengle Scholarship

Our motivation for establishing the Thomas R. "Casey" Stengle Scholarship is two-fold : (1) To continue the support that Casey provided in his passionate love of teaching at UMass for students who were of diverse backgrounds, including many foreign students; and (2) To provide specific support to students who achieve academic excellence with hard work and dedication to their own education.

Casey came to UMass from the University of Michigan, where he studied Raman and infrared spectroscopy, and established the first NMR research facility at UMass, when NMR was in its infancy. His particular interest was in nuclei of inorganic systems, including Xe-131, rather than the trend in later developments ( which established H-1 and later C-13 as the primary nuclei of interest). He believed in the importance of NMR as an analytical/physical chemistry technique. He worked closely with Ken Williamson at Mt. Holyoke, who brought in one of the first C-13 NMR instruments for student use.

Casey's avocation was the outdoors, particularly mountain-climbing, and serving as the advisor to the UMass Outing Club (UMOC). He was instrumental in the procurement of the land and other resources to build a cabin in New Hampshire for UMOC use, and led trips to mountains in Mexico for students in the summer. Casey was a part of a research effort in the Canadian Rockies with the Canadian Air Force in order to study mountain sickness and other effects of lowered oxygen environments, and contributed to published papers in this field. He also was part of a team of climbers who named seven peaks in the Canadian Rockies, including one after Chief Metawampe.

### Thomas R. "Casey" Stengle Scholarship Awardee



Olivia Pietrobuono, Anne Stengle, and Diane Stengle

Olivia Pietrobuono, a rising junior chemistry major, has been rewarded the Thomas R. "Casey" Stengle Scholarship. She says, "Receiving this award has been a complete honor. As an out of state student coming to UMass, at first it was quite a challenge, but having opportunities, such as receiving this incredible award, has made it all worthwhile. Receiving this scholarship means so much to both myself and my family because of the impact it has on taking away some of the financial burden that comes along with college. The scholarship has pushed me to continue to achieve my academic goals. I have a dream of becoming a teacher one day in K-12 schools and this scholarship has allowed me to continue on the path I am on and keep reaching for my goals. I am so thankful to have been selected to receive such an incredible scholarship and will continue to push myself each and everyday. This scholarship has also been an amazing honor because it has proved to me that all my hard work is worth it and to never give up on my dreams."



## ENDOWMENTS

Roger G. Bates Chemistry Fund  
J.F.B. Fund for Undergraduate Research in Chemistry  
Michael Bruno Chemistry Scholarship  
John A. Chandler Memorial Scholarship in Chemistry  
Chemistry Undergraduate Research Scholarship  
Donald E. & Phyllis J. Kuhn Graduate Scholarship in Chemistry  
Richard & Barbara Mahoney Chemistry Fund  
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Charles A. Peters Fund  
Jay A. Pirog Scholarship Fund  
The Professor Jack Ragle Endowed Fund in Chemistry  
Marvin D. Rausch Lectureship in Organometallic Chemistry  
Dr. Richard and Judith Stein Endowed Fund for Sustainability and Renewable Energy  
Edward Shapiro Scholarship Fund  
Dr. Paul Hatheway Terry Endowment  
Robert Maxwell Williams Memorial Scholarship Fund

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Mark D. Argentine '91 MS, '93 PhD  
Robert Austin '67 MS, '68 PhD  
John S. Babiec, Jr. '67 PhD  
Beatrice H. Botch  
Bette Bridges '72 & Kenneth W. Brody  
Margaret Bruno  
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Donald E. Kuhn '70 PhD & Phyllis (Wall) Kuhn '68 MS, '70 PhD  
Robert M. Mahoney '70 & Kathleen Mahoney '70  
Barbara McCarty  
Christopher T. McDevitt '04 & Ana McDevitt  
Donald N. Schulz '71 PhD & Kathleen (Ware) Schulz '70  
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Sravan K. Surampudi '13 PhD  
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Jung-Hsien Tsao '74 PhD  
Anchuu Wu '89 PhD

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Rebecca Bell '81  
Harvey A. Berman '75 PhD  
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Michael J. Clifford '50, '53 MS  
Carolyn (Ives) Dingman '70  
Elinor Goff  
Dennis S. Hackett '76 PhD  
Rajdeep S. Kalgutkar '97 PhD  
Joseph Malgiolio '56  
Thomas H. Mourey '76, '79 PhD  
Brigid O'Brien '02  
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"My research in Prof. Min Chen's lab was the best part of my UMass education. I was able to explore areas that interested me in a deeper way as well as improve my problem solving and critical thinking skills. I am so grateful to the support that I received from Prof. Chen and the lab members, from helping me to learn scientific topics to helping me apply to competitive internships. The knowledge and experience that I gained through my four years in Prof. Chen's lab allowed me to pursue my education in chemistry further in a PhD program at MIT. "

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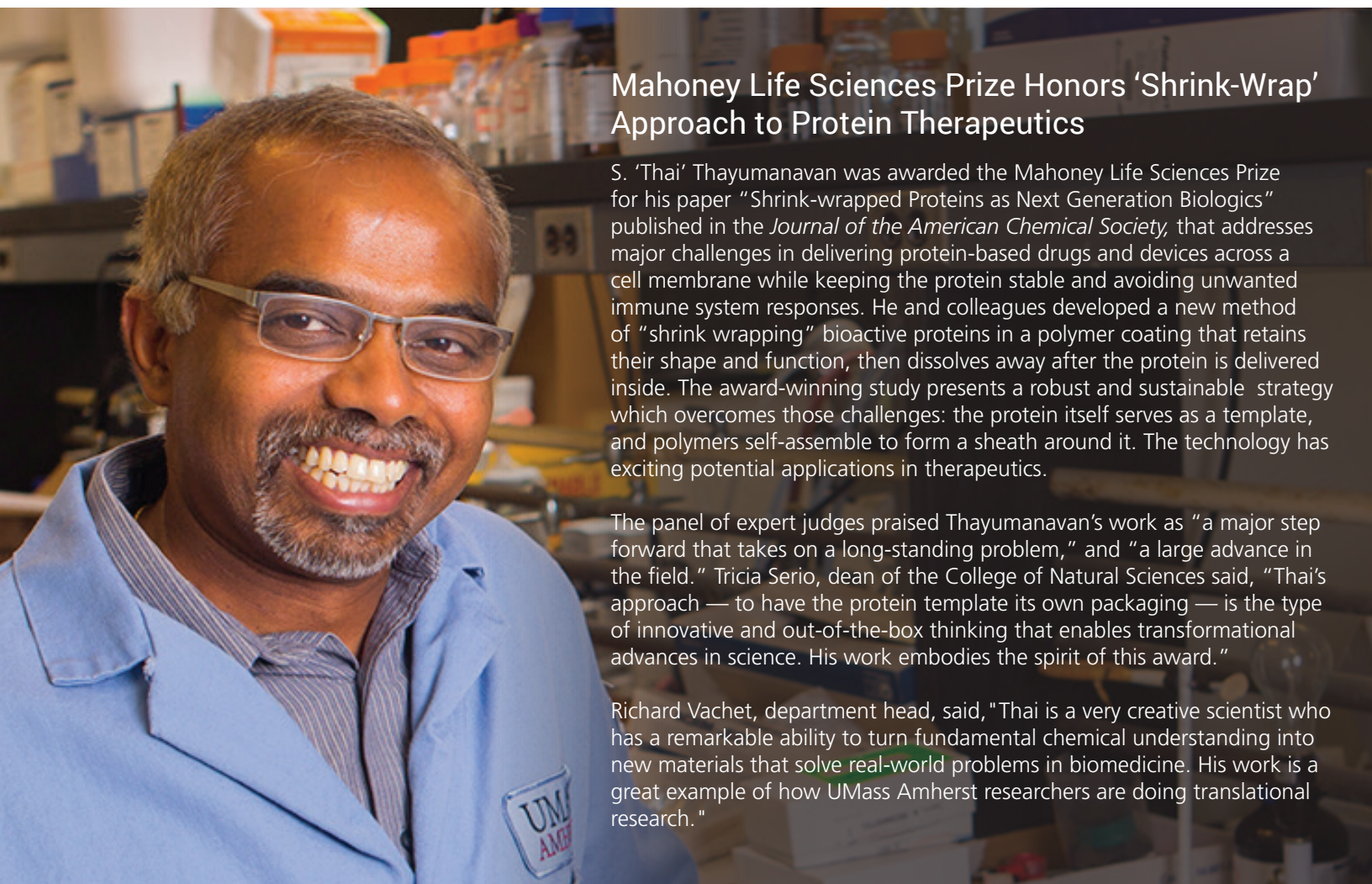
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## Mahoney Life Sciences Prize Honors 'Shrink-Wrap' Approach to Protein Therapeutics

S. 'Thai' Thayumanavan was awarded the Mahoney Life Sciences Prize for his paper "Shrink-wrapped Proteins as Next Generation Biologics" published in the *Journal of the American Chemical Society*, that addresses major challenges in delivering protein-based drugs and devices across a cell membrane while keeping the protein stable and avoiding unwanted immune system responses. He and colleagues developed a new method of "shrink wrapping" bioactive proteins in a polymer coating that retains their shape and function, then dissolves away after the protein is delivered inside. The award-winning study presents a robust and sustainable strategy which overcomes those challenges: the protein itself serves as a template, and polymers self-assemble to form a sheath around it. The technology has exciting potential applications in therapeutics.

The panel of expert judges praised Thayumanavan's work as "a major step forward that takes on a long-standing problem," and "a large advance in the field." Tricia Serio, dean of the College of Natural Sciences said, "Thai's approach — to have the protein template its own packaging — is the type of innovative and out-of-the-box thinking that enables transformational advances in science. His work embodies the spirit of this award."

Richard Vachet, department head, said, "Thai is a very creative scientist who has a remarkable ability to turn fundamental chemical understanding into new materials that solve real-world problems in biomedicine. His work is a great example of how UMass Amherst researchers are doing translational research."