CHEMISTRY

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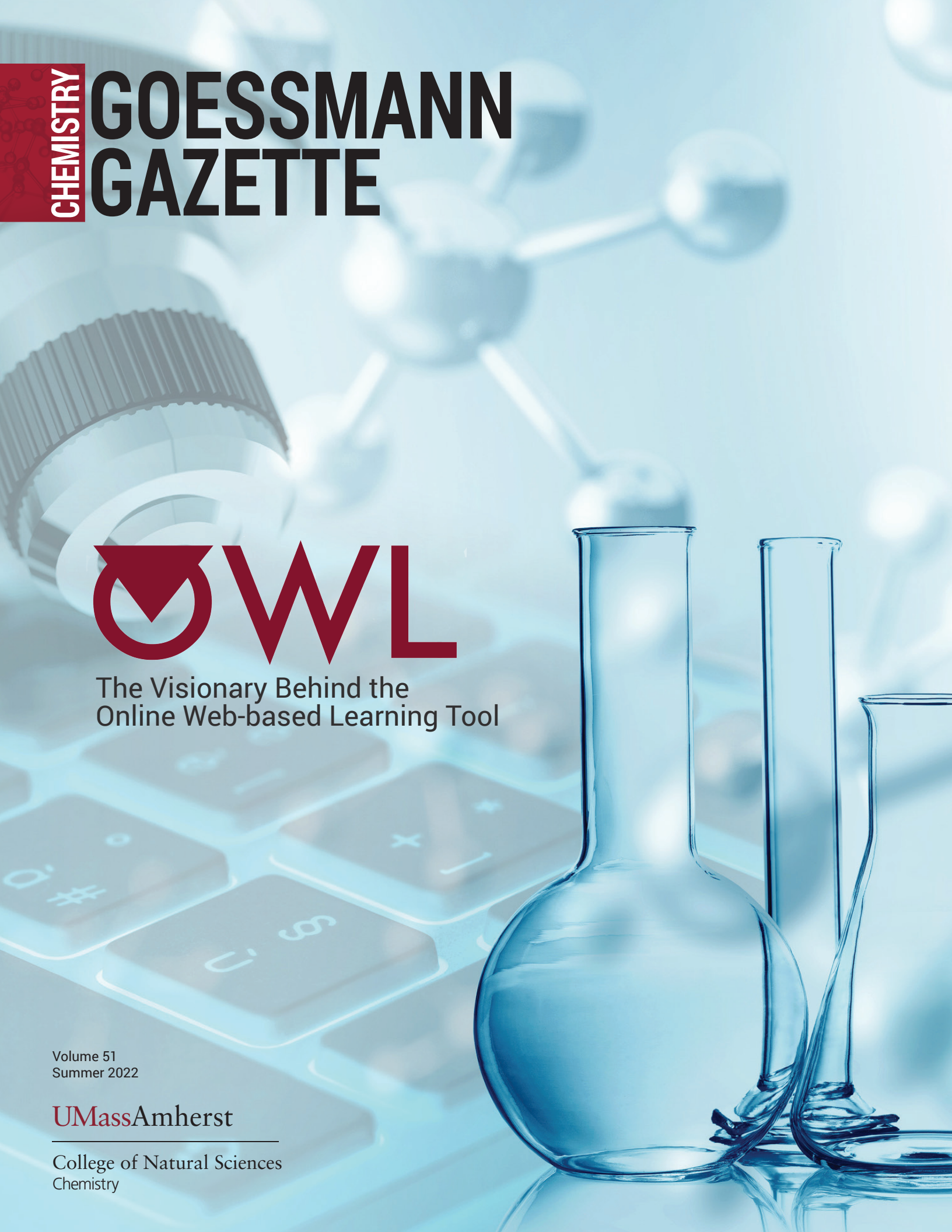

OWL

The Visionary Behind the Online Web-based Learning Tool

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THIS ISSUE

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Dear Alumni and Friends of UMass Chemistry,

Each year, the College of Natural Sciences Outstanding Achievement Awards recognize excellence and honor the faculty, staff, and students in the college who have made important contributions to their discipline, department, college, and university. This year was extraordinary, as four members of our chemistry community were recognized for their outstanding efforts! Graduate Program Manager Rebecca David was awarded the Outstanding Staff Award, Senior Lecturer and Chief Undergraduate Advisor Ruthanne Paradise received the Outstanding Advisor Award, Professor Lynmarie Thompson received the Outstanding Service & Engagement Award, and Outstanding Researcher was awarded to Professor Jianhan Chen. In addition, Assistant Professor Michelle Farkas received the Commitment to Diversity Faculty Award from the UMass Graduate School.

Accolades for our faculty extended beyond campus, with several winning national awards. Professor Lynmarie Thompson was elected a Fellow to the American Association for the Advancement of Science, reflecting her exceptional research accomplishments in understanding the structure and function of membrane proteins. In addition, Professors Michelle Farkas and Jianhan Chen received prestigious NIH Maximizing Investigators' Research Awards (MIRA). Three faculty were promoted, reflecting the excellence of their contributions in research, teaching, and service. Assistant Professors Michelle Farkas and Mingxu You were promoted to Associate Professor with tenure and Associate Professor Eric Strieter to Full Professor. It is wonderful to see the achievements of our faculty and staff be recognized.

We mourn the passing of Professor Emerita Roberta Day and, with remembrances from colleagues, celebrate her contributions to inorganic chemistry and, especially, to the development of the Online Web-based Learning system (OWL), which transformed undergraduate education in our department.

Several graduate students won competitive fellowships to support their research: Michael Lu-Díaz (Donald Kuhn Graduate Fellowship), Enes Buz and Tongkun Wang (PPG Fellowship), Zhining (Jennings) Sun (Paul Hatheway Terry Scholarship) and Xianzhi Zhang (Marvin D. Rausch Fellowship). Undergraduate Ethan French was named a UMass Rising Researcher for his work with Assistant Professor Zhou Lin to develop novel and highly efficient computational chemistry techniques.

It's been wonderful to return to in-person events and celebrations! This made the Senior and Awards dinner, Commencement, and CNS Senior Celebration especially meaningful, and it was inspiring to hear about the academic achievements and exciting research being carried out by our students.

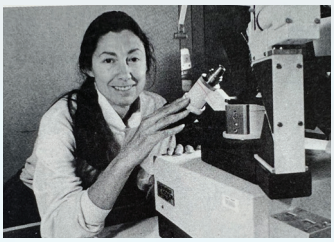
We are deeply grateful to all of you who have contributed so generously to our department over the years. Your gifts contribute to the resilience and growth of the department by providing scholarships to students and improving our teaching and research facilities. With your support, we will continue to train top-notch scientists and advance the frontiers of knowledge! Thanks to you, UMass has great chemistry!

Sincerely,

Ricardo Metz, Head of Chemistry

Roberta Day: the Visionary Behind OWL

compiled by Amanda Bennett



The Online Web-based Learning tool (OWL) has been an indispensable part of teaching and learning at UMass and beyond. Professor of Chemistry Roberta Day, one of the key visionaries and inventors of OWL, passed away this past winter. A few who knew her well shared tributes to Roberta, reflecting on her legacy. Here, they collectively tell the remarkable story of Roberta and the evolution and impact of OWL.

Mike Maroney, Professor of Chemistry: Professor Roberta Ogilvie Day received her BS in Chemistry from the University of Rochester in 1962 and completed her PhD at MIT in 1971, where she worked on nucleic acid crystal structures with Prof. Alexander Rich (of Z-DNA fame). She came to UMass in 1978 for a postdoctoral appointment with Prof. Robert Holmes, where she established herself as a world-class crystallographer. Much of her work at UMass was in support of Holmes' synthetic research program in main group chemistry, particularly phosphorus chemistry, for which she conducted the crystallographic measurements and structural analysis. She was sought out by many, both on and off campus, for her expertise, and she collaborated with many colleagues in the UMass Chemistry Department, including Profs. Marvin Rausch, Ron Archer, Louis Quin, John Wood, John Ragle, and myself. By the time she retired, she had been put on tenure track and promoted to Professor based in part on the strength of her research record, which generated over 200 career research publications, as well as her dedication to teaching.

The Creation of OWL

Peter Lillya, Emeritus Professor of Chemistry: My story begins in the mid 80s when our Department Head, Bob Rowell, went off to China and left me as acting head. Each time this happened, I tried to tackle a serious problem that would be a thorny proposition for someone who had to continue as "permanent" head. This time it was General Chemistry "quiz" sections. In those days every student in a General Chemistry course met weekly with a faculty or TA instructor in a 20 to 30-student discussion section that finished with a quiz. Our teaching assistants and faculty were being "eaten alive" by the time this required.

Many students had no computer in those days, so the committee conceived the "Resource Center," which launched with the newly hired Beatrice Botch as director.

Beatrice Botch, Senior Lecturer II, Retired: It was largely Roberta Day's vision that started the Chemistry Resource Center (CRC). As she tells the story, the committee was tasked with serving more effectively the 1,500+ General Chemistry students we were getting each semester, with fewer faculty and fewer graduate students. *(Editor's note: Gen Chem semester enrollments now exceed 2000.)*

Peter Lillya: Their solution, which we chose to adopt, was to replace in-person "quiz" sections with computer-based learning exercises.

Beatrice Botch: Roberta pioneered the delivery of chemistry homework using the PLATO system from Control Data Corporation out of Minneapolis, long before any major university program (except the University of Illinois, who created PLATO) adopted it. This required entering all of those thousands of "quiz" questions into PLATO on the CDC mainframe, and using small desktop computers as terminals to access the content. By the time I arrived, the CRC had been in operation for three semesters. Thousands of students marched through the Center, open from 1:00 pm to midnight, to do their PLATO homework and to watch the prelab videos for their upcoming lab sessions.

Peter Lillya: It was a challenge to write questions in PLATO; Roberta took this on and became our expert and chief author.

Dave Hart, Director of Enterprise Systems & Development, UMass: The new system they designed within PLATO was not about giving weekly quizzes so much as it was a mastery learning system, encouraging students to do different batches of questions until they got a certain number right. Each question came with explanations of the correct answer so that students were learning from their mistakes as they worked the question sets. The beauty of the system was that getting credit for the assignment (i.e., "passing the quiz") was within reach of every student as long as they applied themselves. At the same time, cheating was minimized because the authors created so many questions that the student rarely saw the same one twice.

Peter Lillya: By the 90s, the limitations and obsolescence of PLATO had become serious.

Beatrice Botch: After an exhaustive search for a replacement system, Linda Slakey, our dean, pointed out that we had the resources on campus to do this ourselves. Roberta and I were sent to talk with Beverly Woolfe in Computer Science to create a new system and migrate off of PLATO. We met with Bev, Dave Hart, and Dave Stemple, Chair of Computer Science. At that historic 1996 meeting, OWL, Online Web-based Learning, was born, well before we really knew what the "web" was or how it would ultimately function. The Center for Educational Software Development (CESD) was formed and their creative team of Bev, Dave, Cindy Stein, Steve Battisti (and others throughout the years), partnered with our creative team of Roberta, Bill Vining, Peter Lillya, Steve Hixson and myself to develop a content delivery system that was independent of platform and adaptable to rapidly changing technology. As content experts, we worked hand-in-hand with the software experts to create a system that instructors could use easily, and from which students could effectively learn General Chemistry.

Bill Vining, Professor of Chemistry, SUNY Oneonta: I came to UMass in the mid-nineties and was welcomed into the most innovative, dedicated, and ambitious group of educators I have ever worked with. At the center of this group were Roberta and Bee, who were both heavily involved in the Chemistry Resource Center and PLATO. At the time, they were nearing completion of the first version of the UMass OWL homework system.

Dave Hart: The goal for the new system was that students be able to easily do their assignments from their dorm rooms or off-campus apartments. In the old system, most assignments were done in the Chemistry Resource Center using specialized

software. An obvious but risky way to do this was to build the system on the new World Wide Web, which was just coming into its own. We were able to port the old system's question database over to the Web and get the system running over the course of a year. However, we ran into problems replacing PLATO's authoring tools, so the chemists could not write new questions. This bothered Roberta more than anyone else – she was looking forward to exploring the new possibilities of the Web and in particular was pushing us to find a way to "parameterize" questions, that is, make some of the questions' variables change from instantiation to instantiation, so two students might see an identical "question" but the numbers or chemical compounds might vary, making it essentially two different questions. Roberta grasped the power this would bring to expand the nature of the assignments and the breadth of material the questions could cover.

Bill Vining: OWL's impact was possible because of wise decisions and targeted efforts made during development. The first and most important is that *homework is for learning; quizzes and exams are for evaluation*. This one decision flows through everything that was built at UMass and used nationally. Once Roberta helped the team adopt that philosophy, you build a system that helps students learn, as opposed to just separating those who know at the start from those that who do not. Before OWL, students would try a question from the textbook and get it right or wrong. If it was graded, they would at best get an idea of what they did and did not understand – a week ago! The OWL philosophy of mastery learning is built on the idea that students start their homework without yet fully understanding the material. They learn by applying what they learn in lecture or by reading and see what they can do with it. The beauty is, if they can't do much, they are not failures – they just have to keep working at it.

Beatrice Botch: Roberta's vision guided the outcome. Static multiple-choice questions did little for learning. We developed fully parameterized questions that may ask about sodium chloride in one instance and potassium sulfate in the next. Every calculation was fully parameterized so that given a starting range for a concentration, for example, the final pH had to be calculated for that specified range. Students could not memorize answers because each question was unique to the randomly chosen initial parameters. We quickly realized that the asking of the question was the easiest part. Fully parameterized, well-written feedback was the real key to helping students use the system for learning. We moved the focus from "quizzing" to mastery learning, where students could try every question over and over again to truly master a concept, each time with a new variation of the question. OWL became the patient teacher, asking the same question again and again, giving a complete answer particular to that instance of the question each time, until the light bulb finally went on.

Bill Vining: Roberta stressed that just telling students they got a question wrong is not good enough. If they don't understand the material, they need to be shown how to solve it, and then be able to try again. This idea of feedback is easy to think about, but an enormous amount of work. The coding required to present the full solution to a chemistry problem at times can be pretty simple, but mostly that is not the case. When I first looked at the coding behind OWL questions, I was amazed. A long page of coding for a one-sentence question and a five-line set of feedback. The tables of randomization data are likewise impressive.

Beatrice Botch: Roberta also experimented with the molecular drawing and grading apps that were eventually brought into OWL. Coming from her crystallography background, she was adamant that General Chemistry students should be able to draw and view molecules. She wrote all of the molecular drawing questions in OWL for General Chemistry, using creative visualization techniques to help students understand molecular structure.

Bill Vining: Presciently, this was before students could easily Google homework answers. The unique, sophisticated degree of parameterization used within OWL (and again, the work to implement it) has helped millions of students learn by not letting them cheat. It is the key to mastery learning, the ability to tell a student, *no, that's wrong, here's how it works, now try again with a different example*. To this day, OWL stands as a rare example of an online system for which students can't just Google the answer. So wise, so ahead of its time.

The Expansion of OWL

Dave Hart: Dean Slakey encouraged us to approach other science departments to offer OWL for their classes, in the hope of providing a better homework experience and also to amortize OWL's costs.

Beatrice Botch: So much of our work was fueled by grants from the National Science Foundation, The US Department of Education (FIPSE), the Dreyfus Foundation, the College of Natural Sciences and Mathematics, the University President's Office, the University itself and others. Roberta was instrumental in helping to write the grants, track down the data, tend to the minutiae, as well as reading and editing each one. Her scientific and educational acumen helped us to keep the focus on student learning, not showy interfaces or complex, unused functionality.

Dave Hart: By this time, the cost of developing and maintaining OWL was becoming a challenge. We submitted grants to the National Science Foundation and the US Department of Education to support making this pedagogical model into a system that could be offered to chemistry departments at other colleges and universities. We submitted three successful grant applications over two years and received almost $1M in funding to take OWL to the next level.

By 2002, the university had been awarded a large grant from the Davis Educational Foundation to expand OWL use in ten additional departments. At its peak, OWL was used in 25 departments across campus, a tribute to the foresight Roberta and others showed in structuring PLATO and OWL the way they did.

Beatrice Botch: Besides the wonderful energy and expertise Bill Vining brought the Department, he also brought a partnership with Harcourt Publishing, now Cengage Learning. We adapted our extensive content in General and Organic Chemistry to over 40 Cengage textbooks.

Dave Hart: UMass received licensing revenue from each sale of an "access code" to a student to use the system. In time licensing revenue supplanted the grant awards that originally helped fund OWL development. At its peak around 2010, Cengage's

OWL chemistry homework was used by 200,000 students in over 200 colleges and universities across the country. UMass granted Cengage a perpetual license to use the version of OWL ca. 2010 in the biggest (at that time) intellectual property deal the UMass system had ever made.

Lisa Lockwood, Executive Program Manager Macmillan Learning: I had the honor of working with Roberta while I was an editor and product manager for Chemistry at Cengage Learning. I worked closely with her and the UMass OWL team for nearly 14 years.

Beatrice Botch: Roberta was the anchor that kept us interacting and improving the content. *She reminded all of us over and over that you can't just let content stagnate. It had to be tended like a garden.* Our partnership with Cengage continues to today, where over 100,000 students per semester use OWL to learn chemistry, 25 years after it was first launched on campus.

Bill Vining: The impact Roberta and the OWL team have had on the education of students nationally is profound. In one sense, the impact is huge simply in terms of breadth. Over two million students at hundreds of universities have used these materials during the over 20 years they have been available.

Dave Hart: She was a visionary, enthusiastic early adopter and adapter of technology for education. She was pedagogically astute, hardworking, paid exquisite attention to detail, and always held herself to a high standard. My development team looked to her for inspiration and guidance as we spent two decades improving and expanding OWL's capabilities.

Lisa Lockwood: To date there is not another learning platform that allows students to practice and learn problem solving to the extent that OWL does. This is due to the extensive authoring that Roberta and the other OWL authors completed. In order for this to be successful, the content needed to be completely accurate, accept all correct answers and offer extensive feedback – no easy task, but accomplished by the OWL team.

Dave Hart: She was always a constant through trying times of system performance problems, grant application deadlines, difficult negotiations with powerful publishing companies, and others. It was an honor to work with her and I feel lucky that I and my staff were able to collaborate with her and the whole Chemistry team on this remarkable, rewarding journey.

Roberta Day retired from UMass in 2002. She passed away on January 4th, 2022.

Mike Maroney: She was trained as an old-school crystallographer and knew the technique inside and out, but was as well known for her dry wit as for her professionalism. She is a co-author on the first paper that I published on work carried out exclusively at UMass. We went on to publish ten papers together. I remember our almost daily conversations fondly.

D. Venkataraman (DV), Professor of Chemistry: Roberta was always excited to learn new things. Once she saw me mount a crystal using a stack of glass slides and play-doh. She was intrigued and wanted to know what I was doing. I demonstrated to her this technique that I had learned from a crystallographer and explained how it ensures that the crystal does not slide to the side of the mounting pin. Immediately, she wanted to give a try and see if it stacks up to the claims I had made. That was Roberta! Always curious and willing to learn.

Lisa Lockwood: Roberta was tireless, committed to excellence, and passionate about helping students master chemistry concepts and realize their potential. Her work on OWL, along with the other OWL authors, touched the lives of millions of students.

Bill Vining: Roberta was an incredibly hard worker, terrifically productive, open minded about better ways to approach a problem, an exceptional chemist, very direct, and she never cut corners. And always, for all the details, I keep reminding myself of that single student, sitting in their room feeling lost working on their homework. And how these materials get them through. Roberta and the team worked really, really hard to do that for those students. I am so proud of them. And thankful to have been part of it.

Peter Lillya: Roberta was the quintessential colleague, eager to talk about what we were doing and how it might better enable learning. When I was unable to author an OWL question to work the way I wanted, she was always willing to show me how. The structure of my questions was less sophisticated than that of hers, and she never failed to solve my problem. Many people in Chemistry deserve some credit for the OWL online chemistry learning system. Several people contributed in unique and essential ways. But Roberta's contributions loom above all the rest. Bee Botch rightfully calls her a visionary.

Beatrice Botch: Roberta was a wonderful, supportive friend. We would spend hours talking about learning, how to better reach our students, how to demonstrate the benefit of the resources we developed. One afternoon, after a particularly long discussion, we realized that the clock in my office had stopped working and we had yacked well past the time when her husband was supposed to pick her up. "Get your clock fixed," she quipped while rushing out the door to make amends.

Dave Hart: Working with Roberta and the entire OWL team has been one of the highlights of my career. To be involved in a 25-year project/journey that innovative and that impactful has been hugely rewarding. Roberta played such a central role that it's hard to overstate her impact. On top of that, however, was her personal impact on us: her dedication, her insight, her drive, her wry sense of humor, her keen sense of fairness, and her compassion. These rubbed off on us and made us a better team, capable of making significant contributions to the Chemistry Department, to campus and to higher education. I miss all of those things about Roberta and I know my team does too.

Bill Vining: Equity and inclusion were not as much thought of 20 years ago. But the philosophy of the materials Roberta spearheaded were based on that idea: some students come to you well prepared, others not so much—through no fault of their own. The mastery system meets all students at the start and gives them the support they need to learn and eventually master the material. The positive impact of this (and all the work to implement it) is humbling to consider. Thousands and thousands of students who would have gotten failing grades on their homework and left discouraged were instead given the opportunity to work their way to a successful level of understanding. There are countless students who became doctors or engineers or researchers, or whatever else they wanted to be, in part because OWL got them through an early tough challenge for which they were not ready. What an incredible legacy.

faculty
Highlights

Auerbach Team Predicting Faster Formation of Nanoporous Material

An interdisciplinary team of UMass Amherst researchers led by chemistry professor **Scott Auerbach** and chemical engineering professor Wei Fan reported breakthrough computer simulations confirmed by experiments showing faster ways to crystallize nanoporous catalysts known as zeolites.

"Understanding how to make zeolites, and how to make them faster, is incredibly important. Zeolites are the most used synthetic catalysts on planet earth, and they show great potential for making green fuels and capturing carbon dioxide — both critical for battling climate change," said Auerbach.

The team also includes Cecilia Bores, a former postdoctoral fellow at UMass Amherst and now a physics professor at Union College, as well as chemical engineering PhD student Song Luo and undergraduate researchers J. David Lonergan, Eden Richardson, and Alexander Engstrom.

"Simulating zeolite crystallization is one of the grand challenges in materials science because the process can take days to weeks, so our simulations have to efficiently model very slow assembly processes," said Bores. She continued, "The key to our work is capturing only the essential aspects of zeolite bonding and intentionally omitting some interactions between particles that would only slow down the simulation."

"Learning how faster zeolite crystallization occurs by using several structure directing agents is a real breakthrough for my lab," said Fan. "We spend countless hours trying to fabricate new zeolites, so being able to speed up the process can lead to much faster discovery of new and useful materials."

Chen Named CNS Outstanding Researcher

Professor **Jianhan Chen** received the CNS Outstanding Research Award in recognition of significant contributions in his areas of research. He has established himself as a national and international leader with 86 published articles and an H-index of 31, according to Google Scholar.

His research group has made numerous contributions in developing advanced computational tools that allow one to simulate large, complex biomolecules and biomaterials with ever-increasing accuracy and efficiency. His research group is also recognized in the development of so-called implicit solvent models, which allow one to perform atomistic simulations of biomolecules without explicitly accounting for water molecules. These methods are expected to be particularly powerful for studying self-assembly of proteins and biomimetic materials.

A central theme of his research is large-scale conformational transitions of biomolecules involved in a diverse set of problems in biology, biomedical engineering and biomaterials. Chen's research group is a leader in studies of intrinsically disordered proteins (IDPs), which are exciting and challenging systems of fundamental biological and biomedical significance. Chen has numerous collaborations with colleagues across campus, who greatly value the insights his simulations provide.

"I am very thrilled to receive this award. It is truly a great honor. I greatly appreciate the encouragement and support of my colleagues in Chemistry and Biochemistry & Molecular Biology. I moved to UMass in 2017, and this past five years have been the best of my scientific career. The intellectual environments here in CNS and IALS are rich and inspiring. I am surrounded by outstanding colleagues with diverse research interests and many exciting ideas. I am also blessed with the opportunity to work with many talented graduate students and postdoctoral fellows. The award is really a recognition of their dedication and collective accomplishments." — Jianhan Chen

Chen's NIH MIRA Grant Will Support Trailblazing Research

Jianhan Chen was awarded a MIRA grant by the National Institutes of Health to focus on using computer simulations to model the molecular structure and dynamics of proteins. Molecular modeling of disordered proteins could lead to cancer drug breakthroughs. "IDPs are a mess; it's difficult to determine the details of their properties because they are not amenable to traditional techniques that are designed to resolve stable protein structures," Chen says.

"This disorder seems to provide some unique functional advantage, and that's why we have so much disorder in certain kinds of proteins," Chen says. "These IDPs play really important roles in biology, and when something breaks down, they lead to very serious diseases, like cancers and neurodegenerative diseases."

Because of their chaotic state, IDPs must be described using ensembles of structures, and computer simulations play a crucial role in the quantitative description of these disordered ensembles. "Our goal is really trying to combine simulation and experiments in collaboration with other labs to tease out what are the hidden features of these disordered proteins that are crucial to their function," Chen says. "Then we can look at how these specific features might be perturbed by disease-related mutations or conditions."

The next step would be to develop effective strategies for targeting disordered protein states. Toward that end, Chen's lab will study the molecular basis of how the anti-cancer drug EGCG, an antioxidant found in green tea extract, and their derivatives interact with p53, a tumor suppressor and the most important protein involved in cancer.

The key, he says, is knowing how to design drug molecules to bind well enough to IDPs to achieve a therapeutic effect. "We believe that targeting IDPs requires new strategies that explore the dynamic nature of IDP interactions," Chen says. "If we can

do this, it could really open up a whole class of drugs that were previously thought impossible."

Farkas Receives NIH MIRA Grant to Study Circadian Rhythms in Cells

Professor **Michelle Farkas** was awarded a MIRA grant by the National Institutes of Health to develop next-generation tools to track and manipulate circadian rhythms in cells, helping researchers to understand the role that such rhythms play in disease.

Circadian clocks help regulate a number of different processes in the human body, including sleep-wake cycles, body temperature, blood pressure, food intake, hormone release, cardiac function, immune responses and metabolism. On the cellular level, circadian clocks also play a role in cellular proliferation, metabolism and DNA damage repair. Though researchers have known for years that changes to the circadian clock's daily rhythms can lead to all sorts of diseases, including various cancers, we don't yet know exactly what is going wrong at the cellular level when the circadian clock is altered.

"We can generate static snapshots of a cell," says Farkas, "but they don't tell you all that much. We need tools to help us track the dynamic changes occurring inside a cell over time." Only then can researchers begin to see what happens when the circadian clock is altered.

Farkas and her colleagues will continue to develop tools, which will allow researchers to watch as proteins are generated by multiple genes at the same time. "These next-generation tools, called 'reporters,' will let us track the process for different components, giving us a clearer, more complete picture."

The group is also generating new approaches to "perturb," or alter, the circadian rhythms of the cells by directly targeting the core circadian proteins. By using their reporters to track the proteins that are at the heart of the cell's circadian clock, the team will be able to alter circadian rhythms and watch how cells respond—including responses that lead to the development of cancer.

Farkas Receives Commitment to Diversity Faculty Award

The award from the UMass Graduate School commends Prof. Michelle Farkas as a tireless advocate for supporting and mentoring students from groups underrepresented in graduate education and notes that she has contributed significantly to advancing diversity and inclusion in STEM, especially among the LGBTQI+ community.

Lin Receives ADVANCE Collaborative Seed Grant

Chemistry assistant professor **Zhou Lin** along with Hui Guan, assistant professor at the Manning College of Information and Computer Sciences, were awarded a 2021–2022 ADVANCE seed grant for their project, "Accelerating Fragment-Based Quantum Chemistry via Machine Learning."

The UMass ADVANCE seed grants, funded by the National Science Foundation, aim to foster the development of innovative and equitable collaborative research projects among faculty, especially women and people from populations underrepresented in science and engineering.

The team will develop computational methods that are hybrids of physics-based and data-driven approaches for modeling electronic and optical properties of many-fragment systems. Many-fragment systems, where fragments are connected through various types of bonds and novel electronic and optical properties are exhibited, are used in many research fields such as computational, medical, chemical, materials and biological sciences that deal with real-life functional molecules or materials.

Currently, the design of these systems often requires trial-and-error experiments that are highly labor intensive. Quantum chemical modeling, which involves building systems based on structural and electronic configurations in molecules, is being increasingly explored as a method for designing many-fragment systems, but researchers have been held back by very high computational costs associated with the method. Their approach will build on their existing work showing that state-of-the-art machine learning algorithms can solve problems inherent to quantum chemical modeling of these systems, proposing to build graph convolutional neural networks to achieve significant computational cost reduction while maintaining performance.

Lin Receives RCSA Scialog: Negative Emissions Science Team Award

Zhou Lin and her co-investigators, Sen Zhang from the University of Virginia and Yayuan Liu from the Johns Hopkins University, received the ("science + dialog") Scialog Negative Emissions Science Team Award from Research Corporation for Science Advancement (RCSA) for their proposal, "Carbon Dioxide-Methane Coupling with Electric-Field-Polarized Microelectrodes." The project aims to develop a new electrosynthetic route that reduces the emissions of two of the most significant greenhouse gases from waste management and treatment activities: carbon dioxide and methane. The grant will help the team design unconventional electrochemical reactors and catalysts to enable direct coupling of carbon dioxide and methane into valuable liquid feedstock acetic acid.

Martin Joins International Team Looking to Revolutionize mRNA Vaccines and Therapeutics

Professor **Craig Martin** will lead a UMass team that will spend the next three years developing a processes that can deliver the quantity and quality of messenger RNA (mRNA) demanded by a new class of medicines, including the COVID vaccines, faster, cheaper, and more effectively than any other method. Martin and his

colleagues will be joining Wellcome Leap's R3 program, which seeks to create a global network of "biofoundaries" capable of producing high quality, low-cost mRNA, increasing global access to these new therapies, wherever they're needed.

"We can make the RNA that encodes the protein, deliver that RNA as the biologic, and the patient's own cells then make that protein from the delivered RNA", says Martin. The result is that, when the body makes the protein itself, "everything gets done correctly" and "once you know how to make the RNA for one disease, it's comparatively easy to swap in a different RNA so it can treat another disease. You don't have to reinvent the wheel, saving money, and, crucially, saving time."

If RNA therapies have not yet reached their full potential, it's because making RNA that is pure enough, in great enough quantities, has proved very difficult—and the purity is of utmost importance. Impure RNA looks to the body's immune system like an invader (though of course it is not) and triggers an immune response that leads to inflammation. "A small amount of inflammation is actually ok for vaccines," says Martin, "because what vaccines do is train the body's immune system to recognize disease." For certain diseases, though, especially those that are caused by genetic deficiencies, and for which the immune system plays no role, purity that fully eliminates inflammation is important. Many cancers, too, are the result of genetic malfunctions, and could be treated with RNA therapies. "In this example, we'll need to generate small amounts of patient-personalized RNA," says Martin.

Martin, whose lab has been studying the enzyme used to synthesize RNA for more than 30 years, has developed an approach to making RNA that employs a "flow reactor," a method that results in much larger quantities of much purer RNA.

Martin Wins Innovation Award

Professor Craig Martin is the team leader for one of six teams chosen by UMass Amherst's Institute for Applied Life Sciences (IALS) to receive the 3rd annual Manning/IALS Innovation Awards. His project, RNA4Therapeutics, a novel manufacturing technology for the synthesis of high purity, low-cost, and large scale RNA manufacturing was selected from a highly competitive group of applicants. These translational grants are designed to advance applied research and development efforts from UMass-based faculty research groups in the sciences and engineering.

Alumnus Paul Manning and his wife, Diane, committed $3 million through their family foundation to establish the Manning Innovation Program. The gift provides three years of support in advancing a robust and sustainable commercialization pipeline of applied and translational research projects from UMass Amherst.

"The Manning Innovation Awards are the perfect catalyst for forging collaborative effort across campus disciplines in support of moving ground-breaking science from our labs to our community," says CNS Dean Tricia Serio. "This investment again supports UMass as a partner of choice in advancing and generating new knowledge, leading to the betterment of society."

Paradise Receives CNS Outstanding Advisor Award

Dr. Ruthanne Paradise is the backbone of our advising team, with her sound knowledge of departmental and university policies, devotion to students, and dedicated support of the chemistry faculty who advise our majors. In addition to being our Chief Undergraduate Advisor (CUA), she is also our New Students Orientation coordinator, organizing faculty advising and materials in summer and winter for our new students. Her approachability, respectfulness, and compassion provide students an excellent introduction to our department.

She created uniformity in our advising by reinventing our departmental advising handbook, making it easier for the ~20 faculty advisors to quickly find appropriate topics and solutions in an interactive electronic format. She has provided additional tools, explanations, and resources for advising faculty to adjust to the shifting platforms. The increase in advising resources and communications has been critical in standardizing our advising, which has been especially important as new faculty members have been brought into the advising circle. Student progress is closely monitored by the advising team, and Ruthanne regularly reaches out to students on more challenging paths. Her experience and empathy for students, along with sound advice, is critical to their success, not only academically, but out of the classroom, as well.

"As the Chief Undergraduate Advisor for the Chemistry department, I care deeply about the students in the program and want to help them find a place to thrive at UMass. I also want to make sure every student is heard and help them to thrive and grow. My life has become more rewarding because of the depth and breadth of students that I have encountered advising in our department and university." — Ruthanne Paradise

Rotello Among Most Influential Global Researchers

Professor **Vincent Rotello** is one of eleven researchers at UMass Amherst to be recognized for being among the world's most highly cited in 2021. Clarivate Analytics identifies researchers who demonstrate significant influence in their fields.

"It is increasingly important for nations and institutions to recognize and support the exceptional researchers who are driving the expansion of the world's knowledge," said David Pendlebury, senior citation analyst at the Institute for Scientific Information at Clarivate. "This list identifies and celebrates exceptional individual researchers at UMass Amherst who are having a significant impact on the research community as evidenced by the rate at which their work is being cited by their peers. The research they have contributed is fueling the innovation, sustainability, health and security that is key for our society's future."

Thompson Elected as Fellow to the American Association for the Advancement of Science

The American Association for the Advancement of Science (AAAS), the preeminent scientific institution in the United States, the world's largest general scientific society and publisher of the Science family of journals, has elected chemistry professor Lynmarie Thompson, and CNS Dean, Tricia Serio, to the newest class of AAAS Fellows. It is among the most prestigious honors bestowed by the scientific community.

The focus of Thompson's work is proteins in the membrane of a cell. Membrane proteins are responsible for many of the cell's processes, from harnessing energy to communicating with other cells and sensing the environment. Her lab investigates chemotaxis receptors that sense the environment and can direct the swimming of bacteria, and form protein arrays in the membrane that are "symmetrical and beautifully complex," as Thompson puts it. Membrane proteins are also the targets for a wide range of therapeutic drugs—and yet their structures and mechanisms remain poorly understood.

Thompson is committed to making science a more inclusive, diverse and interdisciplinary endeavor. Thompson has directed the Chemistry-Biology Interface Program (CBI) for twenty years, during which time it has grown to include over 30 labs in various departments across UMass Amherst, hosts a monthly seminar that draws 70+ attendees per session, and annually provides NIH funding for 12 graduate students to work at the intersection of chemistry and biology. Through both CBI and PREP (the Postbaccalaureate Research Education Program), she works to recruit and retain graduate students from under-represented backgrounds. Thompson has also been tireless in her support of addressing gender inequality in the natural sciences, and her mutual mentoring group for women has become a model at UMass for supporting underrepresented researchers.

Thompson Recognized by CNS for Outstanding Service & Engagement

Professor Lynmarie Thompson was awarded the CNS Outstanding Service Award in recognition of her exceptional efforts and leadership that have enhanced graduate training, improved climate and inclusion for under-represented groups at both the graduate and faculty levels, and fostered the success of interdisciplinary science.

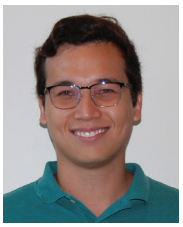
Her leadership as director of the Chemistry-Biology Interface Training Program (CBI) has a major impact on graduate training across multiple departments and programs by providing training opportunities through cross-disciplinary courses and discussion forums. CBI Laboratory Modules have expanded training and usage of the IALS Facilities, providing fundamental training in the Core Facilities.

Thompson has also worked to enhance access to STEM PhD programs for under-represented students in hopes of recruiting them to UMass and to the CBI Program, and helped to design and implement the PREP curriculum. PREP provides students with internships in life sciences laboratories along with coursework and professional development opportunities as a successful bridge to graduate school.

Thompson's work with mutual mentoring groups has had a significant positive impact on climate and inclusion at multiple levels across STEM disciplines. In 2009, she co-founded two mutual mentoring groups for life science women faculty. The experience and advice of these groups has seeded the expansion of mentoring groups across many areas, including graduate students and faculty of color.

"I am very honored to be selected for this award by my colleagues. It has been a privilege to help design and guide programs that help our students and build a vibrant and inclusive research community. I have enjoyed working to enhance training and research at the interface of chemistry and biology, and it's wonderful to see the many positive outcomes, both on campus and in our many successful alumni." — Lynmarie Thompson

graduate student Accomplishments



Lu-Díaz Selected as Spaulding-Smith Fellow for Mentoring & Diversity Program

Michael Lu-Díaz (DV group) was one of three doctoral students selected for the Scientist Mentoring & Diversity Program (SMDP), a one-year career mentoring program that pairs ethnically diverse students and early career researchers with industry mentors in the medical technology, biotechnology, and consumer healthcare industries. Organized by the International Center for Professional Development, this comprehensive program includes a five-day SMDP conference, career development coaching, one year of personalized career mentoring and guidance from an industry leader, networking opportunities, and financial support to attend a major industry conference.

Michael chose to join the SMDP MedTech cohort to learn more about careers at the intersection of science and business. Michael created a mentoring plan with his mentor, a Senior Director of Regulatory Affairs, and the pair met monthly to discuss his progress. "SMDP is a well-structured program that aims to develop rising industry leaders through professional development, networking, and one-on-one mentoring. Now that I have a clear picture of the industry landscape, I have decided to pursue a career in intellectual property at the intersection of science, business, and law," Michael says. This summer, Michael will complete a Technology Specialist internship with Wolf Greenfield & Sacks, a firm that specializes in patent law.

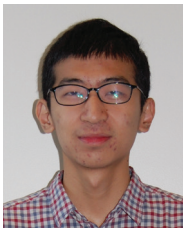
Lu-Díaz Awarded Donald Kuhn Graduate Fellowship

Michael Lu-Díaz (DV group) was awarded the Donald Kuhn Graduate Fellowship for outstanding research, and an interest in pursuing a career in research or teaching.

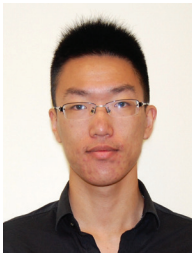
Research Summary: Chemically doped conjugated polymers comprise a myriad of applications among organic electronics. The chemical doping process consists of introducing a molecule to partially oxidize or reduce a polymer's backbone and create a charge. Although this charge is presumed to be mobile, it experiences a strong, attractive Coulomb interaction with a dopant, ultimately affecting charge transport. I am studying methods to screen this Coulomb interaction and help this charge move. Our experiments and models indicate that the dielectric permittivity is a tunable and crucial parameter to reduce polymer-dopant Coulomb interactions. We used a charge hopping model and fabricated polymer composites with nanocrystals with tunable dielectric permittivity. Ongoing studies focus on understanding how different physical properties of a polymer impact polymer-dopant Coulomb interactions to create more efficient materials.

Buz and Wang Receive PPG Fellowships for Outstanding Research in Materials Chemistry

Enes Buz (Kittilstved Group): Transition-metal doped metal oxide semiconductors, in particular $Zn_{1-x}M_xO$, have attracted tremendous interest as potential candidates not only for the semiconductor-compatible magnetic components for spintronic applications but also room-temperature magnetism. While ZnO is a diamagnetic semiconductor, introduction of magnetic dopants such as Fe imparts magnetism on ZnO. In the Kittilstved research group, I study different methods to tune the oxidation state of Fe dopants in ZnO nanocrystals (NCs) in a controlled way which will allow us to control the properties of ZnO NCs in turn. With the support of the PPG fellowship, I will be furthering my studies to investigate and directly show the specific oxidation state of Fe in ZnO NCs by utilizing various dopant-specific spectroscopic techniques. This study will help us to shed light on the mechanism of magnetism in ZnO NCs and to develop materials of interest for magnetism-related applications.

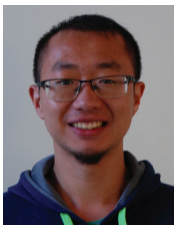


Tongkun Wang (Auerbach Group): Research in Scott Auerbach's group focuses on the study of zeolites, which are atomic crystals formed by tetrahedral atoms like Si with bridging atoms like O. As noticeable members of molecular sieves, zeolites have interesting porous structures and channels. To better understand their formation mechanism, we performed periodic density functional theory simulations and probed key precursors. Combined with experimental results from our collaborators, we successfully used Raman spectroscopy and thermodynamics calculations to reveal defects and explained why or why not they can be healed with the presence of organic structure directing agents. In future works, I will extend my ab initio molecular dynamics simulations in aqueous environment and study processes from monomers, via important building units, to full crystalline, which will help us to predict and design the synthesis for zeolites we want.



Sun Receives Paul Hatheway Terry Scholarship

Zhining (Jennings) Sun (You group): Genetically encodable RNA-based fluorescent sensors have been a revolutionary tool for real-time imaging of important biological small molecules in live cells. Guanosine tetraphosphate (also known as ppGpp or "Magic Spot") in particular is one of the targets that plays an integral role in cell regulation. Its presence in bacteria cells triggers the stringent response which helps the cells to survive the harsh living conditions via various pathways. Although much research has been done to study its functions, people still have not been able to fully understand it due to the lack of tools to monitor it in live cells. I engineered a naturally occurring ppGpp riboswitch into an RNA-based fluorescent sensor and achieved imaging of ppGpp in live E. coli cells. After half a century since its discovery, we are the first group to ever visualize ppGpp and provide information on its cellular dynamics and cell-to-cell variations. Now I'm working on the multiplex imaging project to study ppGpp and other related targets simultaneously, which will discover the potential correlation between the targets as well as how they affect the cell biology.



Zhang Receives Marvin D. Rausch Fellowship

Xianzhi Zhang (Rotello group): Bioorthogonal chemistry uses abiotic chemical processes to create a new toolkit for biological and biomedical applications. Bioorthogonal catalysis via transition metal catalysts (TMCs) provides a particularly promising direction that employs the high catalytic activity and chemical specificity inherent in TMCs. The direct application of TMCs in living cells is challenging due to the generally poor water solubility and instability of these hydrophobic catalysts in biological environments. In the Rotello lab, these issues can be addressed by incorporating TMCs into nanomaterials to generate bioorthogonal "nanozymes." Nanozymes can activate imaging and therapeutic agents from their inactive precursors, creating on-demand "drug factories." By engineering surface functionality and size of nanomaterials, I synthesized various nanozymes with biostability and/or stimuli responsiveness. Furthermore, I also designed and synthesized a library of substrates for nanozymes to broaden their applications for bioimaging, cancer chemotherapy and immunotherapy. The therapeutic potential of nanozymes was demonstrated both in vitro and in vivo, creating an anti-cancer treatment with increased efficacy and reduced side effects.

Equity, Diversity, and Inclusion

Promoting Equitable and Inclusive Practices by Michelle Farkas

From its initiation, the Chemistry Department's Diversity, Equity, and Inclusion (DEI) Committee has sought to improve the climate of the department through various programs and initiatives, involving (and reaching out to) current faculty, staff, and students. This year, Profs. Richard Vachet (committee chair) and Michelle Farkas (committee member) extended that reach to include prospective graduate students who had been offered admission to the chemistry program. As part of the 'in-person' and 'virtual' recruiting weekend events, held on March 4/5 and 11/12, respectively, Profs. Vachet and Farkas spoke to prospective students about DEI efforts in the department and university, including the Chemistry DEI committee, interest/affinity groups, and campus resources. Prospectives were also greeted by Associate Dean for Inclusion and Engagement, Prof. Wilmore Webley. We hope that these discussions continue to be a part of recruiting weekends in the future to promote more equitable and inclusive practices in our Department.

ACS Bridge Program by Michael Knapp and Lynmarie Thompson

Since 2019, UMass Amherst Chemistry has been participating in the ACS Bridge Program which aims to diversify the graduate student population in the chemical sciences. We are excited to report that last summer our program was awarded funding to support two Bridge Scholars per year! The mentorship program, part of the NSF INCLUDES Alliance: Inclusive Graduate Education Network (IGEN), provides additional pathways for Black, Latino, and Indigenous students to receive doctoral degrees. The program is flexible, to match the needs of each student, and applicants are admitted to one of two tracks: the Research-intensive track and the Rotation track. The Research-intensive track is a two-year program leading to a thesis-based MS degree, and the Rotation track is direct admission to the Chemistry PhD program for students who have already had significant research experiences.

All BRIDGE students benefit from opportunities for professional development and community building. Students are invited to an on-ramp program in August to facilitate the transition to UMass and the Amherst community. Students join a research group, take typical first-year courses, have near-peer mentors from the Chemistry graduate program, and are invited to BRIDGE and Chemistry department social activities.

Staff News

Rebecca David Receives Outstanding Staff Award

Rebecca David has earned an exceptional level of respect by all who interact with her. She is efficient, effective, and careful in everything she does, always looking for ways to do her job even better and to be more helpful — planning and organizing for future needs, or devising ways in which we can improve.

Her willingness and ability to step up for the good of the College is particularly noteworthy, as she served as interim Chemistry Graduate Program Manager before being hired into the role, and continued to cover Head's Assistant duties until that position was filled. Rebecca has worked to include more DEI resources and discussion opportunities for graduate students. She is an exemplary staff member who shows great care, professionalism, and patience in everything she does.

"Thank you for this award. I am truly honored to receive it. It means so much to be placed in such distinguished ranks as those of the past honorees. Being a part of the Chemistry Department and CNS has provided me opportunities to learn, grow, and succeed as an individual and as a colleague. Synergy between faculty, staff, students, departments and the college is just one aspect that helps make my work life genuinely enjoyable. UMass does have Great Chemistry. The guidance and encouragement gifted to me means more than I know how to express. You have my immense thanks for all the support and confidence you've given me." — Rebecca David

New Staff

Two new staff members, Allie Lopez-Swetland and Cheng Song, joined the department.

The department welcomed **Allie Lopez-Swetland** as our new Head's Assistant in February. She majored in anthropology as an undergraduate here at Umass and went on to complete a Master's in plant and soil sciences at the Stockbridge School of Agriculture. Allie previously worked for the Massachusetts Department of Agricultural Resources in Amherst, focusing on the export of agricultural plants and surveys of crops, soils, and wild plant species.

Allie takes over the role of Head's Assistant from Rebecca David, who is now our full time Graduate Program Manager. We thank Rebecca for her excellent work as Head's Assistant, which she continued while also serving as our Graduate Program Manager.

Cheng Song joined the Thayumanavan lab as the faculty assistant in the fall. Cheng has been a Polymer scientist and Chemist for more than 15 years. She lives with her two children in Amherst. Last year she initiated a career change to become a faculty assistant in order to take care of her family. She serves on the Amherst Tritons Swim Team (ATST) Board of Directors. Cheng enjoys music, swim, playing poker, cards, and chess.

lab Notes

Auerbach Group

The Auerbach group thrived returning to face-to-face academics during 2021-2022 in research, teaching, and administration. A common thread through **Prof. Auerbach's** teaching and leadership this year was his role in Chancellor Subbaswamy's "UMass Carbon Zero" initiative – transitioning UMass Amherst to net-zero carbon emissions by the year 2032. Such a transition is no small feat considering that UMass Amherst is the biggest emitter of carbon dioxide of all Massachusetts state agencies. UMass Carbon Zero was officially announced on Earth Day 2022, including Prof. Auerbach's participation via his teaching and leadership of the UMass iCons Program. In iCons, a dozen teams of sophomores and juniors across several Business and STEM majors designed solutions for moving UMass closer to net-zero emissions. The fruits of all this labor were showcased at the inaugural UMass Energy Transition Symposium, which was spearheaded by Auerbach along with colleagues in the UMass Energy Transition Institute, and which brought together energy and climate researchers and activists across UMass and beyond. All in all, the "net-zero future" is bright at UMass Amherst as long as we apply pressure on our elected officials to make wise and courageous investments.

Present members of the Auerbach group had a banner year in research during 2021-2022, including the publication of a "hot article" in the journal *Physical Chemistry Chemical Physics* (**Dr. Cecilia Bores**, first author, now a physics professor at Union College) entitled: "Monte Carlo Simulations and Experiments of All-Silica Zeolite LTA Assembly Combining Structure Directing Agents That Match Cage Sizes." Using computer simulations to predict crystallization rates of zeolites is entirely unprecedented, explaining the attention this article has received. In addition, Chemistry PhD student **Tongkun Wang** won a PPG graduate fellowship in recognition of his excellent computational chemistry research in materials science, shedding light on a "3rd route to zeolite formation" in an article in *Chemistry of Materials* entitled: "Titrating Controlled Defects into Si-LTA Zeolite Crystals Using Multiple Organic Structure-Directing Agents." And we congratulate **Dr. Babgen ("Bobby") Manookian** for completing his PhD; see the picture of the happy graduate next to Auerbach and the Armenian flag. We are very proud of all these accomplishments and look forward to further breakthroughs in the coming months.

Prof. Scott Auerbach and Dr. Bobby Manookian next to the Armenian flag at graduation, May 13, 2022

Past members of the Auerbach group are also thriving. For example, **Dr. Usha Viswanathan** (Chemistry PhD, 2012) took a new job in Computer-Aided Drug Design at Johnson & Johnson. We wish Dr. Viswanathan great success in her new position. In addition, **Dr. Harikrishnan Ramanan** (Chem. Eng. PhD, 2004) has taken a new job as Director of Research and Development at Ohmium International, Inc.; Dr. Ramanan's new role involves leading efforts in a new R&D center at the IIT Madras Research Park in Chennai, India for next-generation methods of producing green hydrogen as a chemical and a fuel. We wish Dr. Ramanan great success in this critical endeavor.

In closing, we wish all Auerbach group alums a wonderful year, and we hope you stay in touch and have a good year coming out of the COVID-19 pandemic into a brighter future.

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 (extended through June 2022). The Barnes group also had two papers published as corresponding author, one in *ACS Applied Materials and Interfaces* describing the electronic modification of graphene sheets overlaid with zwitterionic polymers, and a second paper in *Journal of Physical Chemistry Letters* describing the effect of fluorinated polymers on photoluminescence properties of Molybdenum Disulfide 2D sheets.

Nick Hight-Huf has finished his 5th year of graduate studies in the group, and will be defending his thesis later this year on the application of electric-force scanning probe techniques to probe electronic properties in hybrid organic-inorganic two-dimensional nanomaterials. **Nick Heller** (BS Chemistry 2021) finished his undergraduate research thesis on photoluminescence properties of 2D materials coated with zwitterionic polymers. Nick joined the cohort of Chemistry graduate students at CalTech in Fall 2021. **Sarah Marques** (PhD 2019 "Tuning H/J aggregation in organic semiconductor assemblies") finished a postdoctoral fellowship at Georgia Tech in 2021. **Peijian Wang** (PhD Physics, 2018) is currently a postdoctoral researcher in the Physics Dept. at University of Buffalo. **Joelle Labastide** (PhD 2015 "Photophysics of semiconductor aggregates") was awarded a AAAS Policy Fellowship in Washington, DC. **Kevin Early** (PhD 2010 "Photophysics of hybrid quantum dot-conjugated organic nanostructures") is a Senior Project Manager at Illumina Corporation based in San Diego, CA. **Michael Odoi** (PhD 2010 "Time-resolved Single-Molecule Spectroscopy of Semiconductor Quantum Dot-Conjugated Organic Hybrid Nanostructures") leads a product development team at Perkin-Elmer Corp. in Bridgeport, CT. **Austin Cyphersmith** (PhD 2012 "Probing effects of orientation on the chiroptical properties of single molecules") is now a Microscopy and Imaging Laboratory Manager

at University of Illinois-Urbana Champaign. **Ruthanne Hassey Paradise** (PhD 2009, "Chiroptical Spectroscopy of Single Molecules," is a Senior Lecturer at UMass Amherst, and supervises the Analytical and Physical Chemistry Laboratories for undergraduates.

J. Chen Group

This past year, we were thrilled to finally welcome our new graduate student, **Jian Huang**, to UMass after a year's delay due to COVID-19. **Samantha Schultz** continued to work as a Research Assistant after she graduated from Biochemistry early and with honors in Winter 2021. She will stay in the lab for at least one more year for her Master's degree after a summer internship in a biotech company. **Ryan Pham** received his BS in Chemistry this summer and will join the PhD program at Boston University. We all wish him the best luck and are confident that he will be successful there. **Mahdieh Yazdani** and **Xiaorong Liu** came back to visit the lab during Thanksgiving in 2021. We had our own hooding ceremony and they were able to share some precious experience and wisdom on how to better prepare for academic and industry careers. We also congratulate **Debabani Ganguly**, a former postdoc from the lab, on her promotion to Associate Professor at the JIS Institute of Advanced Studies and Research in Kalkata, India. In Spring 2022, the whole lab except Zhiguang attended our first in-person conferences since the pandemic in San Francisco. Everyone had a great time. This summer, we welcome two new undergraduate students, **Anik Dey** from Amherst College (Biochemistry) and **Jack Madden** from UMass (CS/Pure Math), to the lab.

J. Chen lab mini-reunion, November 2021

The group continued to make exciting progress on several active projects in the general areas of computational biophysics and biomaterials this past year. The group has published several original research and review articles on a diverse set of topics including new molecular models, sampling methodology, intrinsically disordered proteins, protein aggregation, ion channels, protein-ligand interactions, and protein-based biomaterials and nano-devices. Several of these papers have appeared in prestigious journals, including *Nature Communications* and *PLoS Computational Biology,* and receiving substantial media attention. The full list of publications can be found on the lab webpage at: http://people.chem.umass.edu/jchenlab. We have also received a new 5-year NIH R35 MIRA award to support our research on studies of intrinsically disordered proteins. Jianhan was recognized with the CNS Outstanding Award in Research in the Senior category. **Erik Nordquist** was selected as a 2022 CNS Teaching Fellow, to support his efforts in designing a new seminar course for the incoming first-year undergraduate students on a topic of his choice.

M. Chen Group

The Chen group continued the work on developing nanopore-based technologies for disease biomarker sensing, DNA and protein sequencing, and single-molecule enzymology and drug screening.

In May 2022, we celebrated the graduation of Chemistry undergraduate students **Ryan Pham** and **Nhu Tong**, who will start their new journey as graduate students at Boston University and UC Davis, respectively. We wish our alumni a lot of success and happiness in their careers and life!

The Chen group (current graduate students: **Fanjun Li, Spencer Shorkey**, **Joshua Foster**, **Minji Kim**, **Kaitlyn Gilliam**, **Crystal Rodriguez**, **and Jackie Sharp**) had a productive year in 2022. **Fanjun**'s work on applying nanopore tweezers for watching the kinase has been accepted in *Nature Communications*. **Monifa**'s new design of OmpG sensor for detection of ssDNA was published in *Biophysical Journal*. In collaboration with Dr. Olgica Milenkovic at the UIUC, **Bach**, and **Spencer** published a work aiming to "expand the molecular alphabet of a DNA-based data storage system" in *Nano Letters*. We also co-authored a paper on OmpG folding in *Proc Natl Acad Sci USA* with Dr. Mark Wallace's group at Kings College London and a manuscript about bacterial conjugation accepted in *Nature Microbiology* with Dr. Gad Frankel's group at Imperial College London. We are filing a patent application to cover **Joshua** and **Minji**'s invention that has created a multiplex OmpG sensor for antibody screening and quality control. **Katie** has established a method to study intrinsically disordered proteins. **Crystal** has successfully passed the Prospectus exam in the Chemistry PhD program. She is working on a project aiming to improve the accuracy of the current nanopore DNA sequencing technology. We welcome our newest member: MCB graduate student **Jackie Sharp.** Jackie

will be working on nanopore tweezers to study enzymes' motions. Projects in our lab are supported by multiple federal grants from NIAID, NIGHRI, and NIFA/USDA. Our lab has recently attracted two-year industrial funding from Oxford Nanopore Technology, UK, to co-develop sensing tools for disease diagnosis and drug screening. The Chen group is looking forward to a great year in 2023!

DuChene Group

The DuChene Group is now fully settled into our beautiful lab space on the first floor of the new Physical Sciences Building. Despite continued setbacks due to the lingering effects of COVID-19, our lab is making great progress towards the development of new catalysts for the sustainable synthesis of fuels and chemicals. One aspect in which we have been very successful is in the recruitment of new students to the group, as our lab has grown tremendously! We welcome the arrival of two new graduate students, **Ben Adams** and **Lauren McDonald**, to the DuChene Group this year. Ben has been hard at work developing new synthesis strategies for the light-driven synthesis of Cu nanoparticles and has made significant progress on expanding our capabilities for harnessing light to grow catalytic nanomaterials. Lauren has begun her work on developing new strategies for the electrochemical synthesis of well-defined catalytic nanomaterials and will use these approaches for the construction of new spectroscopic platforms for monitoring catalytic reactions *in operando*.

The DuChene has also been joined by many new undergraduate researchers in the past year. We welcome **Sean Bhambhani**, **Erika Brown**, **Owen Doyle**, **Brian Her**, **Wenwei Liang**, **Gavin Maenzo**, and **Bella Pomeroy** to the group. Our undergraduates have made important contributions towards the development of synthesis strategies for electrocatalytic nanomaterials and our understanding of electrochemical processes occurring on these catalysts. We are also very proud to report that two of our group members received undergraduate research awards for their efforts! Erika Brown was the recipient of the Edward Shapiro Scholarship Award and the Undergraduate Research Award, while Owen Doyle received the ACS Analytical Chemistry Award. We also congratulate our graduate student **Rakesh Sahoo** for winning a Chemistry Department Teaching Award for his outstanding contributions to the department's teaching mission! Finally, we would like to acknowledge the hard work of a few of our undergraduate researchers who have recently graduated with their BS degrees: **Bohan Feng**, **Alexander Gauthier**, **Wenwei Liang**, and **Nicole Mamonis**, who successfully defended her undergraduate honors thesis on the shape-controlled synthesis of silver nanoparticles. The DuChene Group sincerely appreciates all their contributions to the group, and we wish them well in their future endeavors!

Farkas Group

The 2021-22 academic year was a very exciting one for the Farkas Lab. Prof. Farkas and the lab were excited and grateful to receive a Maximizing Investigators' Research Award (MIRA) from the National Institutes of Health to pursue their development of chemical tools for studying circadian rhythms. After a year of online teaching during 2020-21 (due to COVID-19), Prof. Farkas became (re)acquainted with the trials and tribulations of teaching 'in-person,' but was glad to be back in the classroom. The first two PhD graduates from the group (**Joseph Hardie** and **Huei-Hsien 'Tanya' Lin**) each had their final first author manuscripts from their UMass careers published – congratulations to them both! Also in graduation news, **Sujeewa Lellupitiyage Don** completed his dissertation ("Tracking and Modulating Circadian Rhythms in Cell Culture Models") during the Spring semester, and promptly started in a Scientist position with Excision BioTherapeutics in Cambridge, Mass. Sujeewa has the honor of being the first Farkas group PhD student to be 'officially' hooded at UMass Graduation in May. Along with his wife Nishadi, he is expecting a baby in early summer – we wish them the best of luck!

Graduate students **Bishnu Joshi** and **Javier Mas-Rosario** are both slated to complete their respective dissertations this summer; it's definitely graduation season in the group! Third year graduate student **Kyle Winters** passed his Original Research Proposal (ORP) examination, making him a PhD candidate, and all three second years in the group, **Bhavna Kalyanaraman**, **Emmanuel Rivera Iglesias**, and **Claudia Yan** completed their prospectuses. We are also excited that Emmanuel received an NIH-funded Chemistry Biology Interface (CBI) Training Fellowship – congratulations!! Prof. Farkas continued to play valuable roles in the department, via serving on the Diversity, Equity, and Inclusion (DEI) and graduate admission committees, seminar hosting, and assisting in the recruitment of top-notch graduate students. She also received the 2022 "Commitment to Diversity Award" from the Graduate School at UMass Amherst. In undergraduate news, we said good-bye to two outstanding undergraduate students – **Maya Hegde** and **Mary Jeffway** (both Biochemistry & Molecular Biology); Maya defended her honors thesis on tracking circadian rhythms in May. Lastly, we are excited for two rising seniors in the group who have secured

outstanding summer research fellowships – **Chris Dahlke** (Biochemistry & Molecular Biology) has received an award from the Connecticut Valley Section (CVS) of the American Chemical Society (ACS) to perform research in the lab, and **Bao Le** (Chemistry) was accepted to the Summer Undergraduate Research Program at the University of Texas MD Anderson Cancer Center.

Hardy Group

The Hardy Lab has enjoyed a year of full-capacity research spaces, in-person classes, and group meetings. We have especially enjoyed seminars, CBI chalk talks, the Biotech tAles, Laboratory Modules, and graduate recruiting in person!

In May, **Ishan Soni**, who published two first-author papers this year, defended his dissertation and graduated in the May Commencement. Ishan is also working on his third first-author paper which features an ongoing collaboration with Roivant Sciences using HDX-MS constraints to calculate protein structure. Undergraduate researcher **Ethan Goulart** also received his baccalaureate in the May 2022 Commencement. Ethan had an exceptional year winning eight departmental awards, including the ACS Organic Chemistry Award and the Royal Society of Chemistry Certificate of Excellence which recognize both his research and scholarship. Ethan's accomplishments are also externally recognized. Ethan was accepted to every PhD program he applied to, including: Harvard, MIT, Princeton, UC Berkeley, University of Illinois Urbana-Champaign, University of Wisconsin Madison, and Yale. He will matriculate into the Chemistry PhD program at UC Berkeley in the fall. Two other undergraduate researchers have both excelled this year as well. Both **Alanna Mahar** and **Grace Baron** were invited to serve as undergraduate TAs in the General Chemistry and Organic Chemistry programs.

Alanna was also honored with the John A. Chandler Memorial Scholarship. Grace won the Anna J. Harrison award for her poster at the ACS Connecticut Valley Section Poster session.

Hardy lab recruited an outstanding new PhD student this year, **Trisha Brady** who will be jointly advised by Prof. Richard Vachet. Trisha joins us from University of New Haven, where she worked in the lab of another UMass alumna **Alyssa Marsico** (Vachet lab). **Rashad Baker**, a 2nd year student, was named a CBI fellow, won the "Hello Cleveland" award for his presentation at the Pacific Coast Protease meeting and also successfully passed his prospectus on identifying exosites responsible for the interaction between caspase-6 and DJ-1. **Nathanael Kuzio** passed his ORP and has made great strides toward NMR-based studies of caspase-6 dynamics and structure. Nathanael was also named "Honorable Mention" for his NSF Graduate Research Fellowship Proposal. **Sparsh Makhaik** led the Hardy lab contribution to a joint project to create a colormetric SARS-CoV-2 swab test in collaboration with the Andrew and Thayumanavan labs. **Irina (Niña) Sagarbarria**, has made significant progress working on determining the structure of caspase-6 with an inhibitor that could be a potential therapeutic for Alzheimer's Disease. In June, she attended the CCP4/APS Virtual School in Macromolecular Crystallography and in July, attended the 36th Annual Symposium of The Protein Society in San Francisco. **Andrew Smith** is investigating interactions between caspase-6 and tau with the goal of finding exosites that may be exploited to develop therapeutics for Alzheimer's Disease. He is making great strides to discover novel exosites on caspase-6 and its substrates, and won the "Too Honest" award at the Pacific Coast Protease meeting. **Kristalle Cruz** is investigating a Zika virus protease inhibitor that we hope may lead to a Zika antiviral and contribute to our understanding of pan-viral inhibition.

Kaltashov Group

2021 was a very busy year in the Kaltashov laboratory. The group continued working on the project that was initiated soon after the onset of the COVID-19 pandemic and focused on the ability of various polyelectrolytes to prevent SARS-CoV-2 fusion with the host cells. A new graduate student, **Kevin Cheung**, and a post-doctoral fellow **Dr. Si-Hung Le** have joined the group. **Yang Yang** successfully defended his PhD dissertation in September 2021 and joined Biogen (Cambridge, MA). A visiting scientist **Dr. Wenhua Yang** (Yichun University in China) finished a two-year stint in the lab and returned home to resume his work at Yichun University. A monograph "Mass Spectrometry in Biopharmaceutical Analysis" co-authored with two former graduate students, **Dr. Shunhai Wang** (presently at Regeneron) and **Prof. Guanbo Wang** (presently at Peking University) was published in December 2021.

In group alumni news: **Mingxuan Zhang** (PhD 2007) become a Senior Director of Analytical Development at EQRx, a company devoted to making protein therapeutics more affordable for oncology patients who need them. This career move follows Mingxuan's successful work as a Director of Large Molecule Analytical Development at GSK (GlaxoSmithKline).

Kittilstved Group

During the 2021-2022 academic year, Kevin and his group saw glimpses of the light at the end of the pandemic tunnel… research labs were more or less operational which led to some exciting discoveries in the multifunctional inorganic

materials chemistry lab. Third year students **Gaurav Mitra** and **Hyunggu Kim** successfully defended their Original Research Proposals, becoming PhD candidates in Fall 2021. They joined PhD candidates **Enes Buz**, **Haneen Mansoor**, and **Jillian Denhardt**. In April 2022, second-year student **Taylor Marcotte** successfully defended his Prospectus on a new project in the group on synthesizing zirconium-based metal oxide nanocrystals for solution-processable soft-hard hybrid materials.

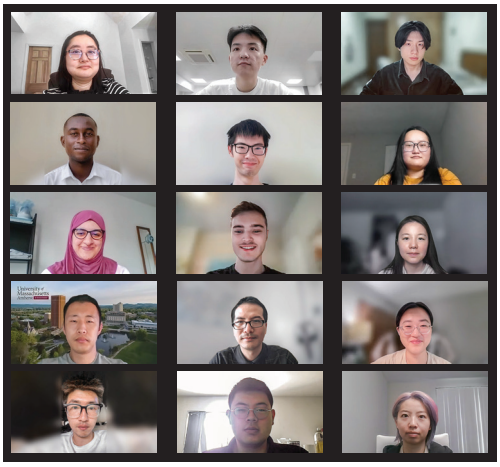
In April 2022, **Jillian Denhardt** successfully defended her thesis on the "Formation of doped semiconductor nanocrystals from doped molecular clusters." Dr. Denhardt developed new synthetic methodologies to introduce dopant ions into precise locations within small "magic-size nanoclusters" with approximate compositions of $(CdS)_{13}$. This work was critical preliminary data for a recently awarded NSF proposal to use these doped magic-size nanoclusters with dopant ions situated at precise locations within the lattice. We are thankful to Dr. Denhardt's contribution to this work and truly paying it forward, giving others an opportunity to continue this awesome work.

The group also welcomed **Moshood "Mo" Animashaun** to the group. Mo started at UMass in Fall 2021 after obtaining his Bachelor's degree from Susquehanna University in biochemistry. Mo will join the clusters project with Hyunggu.

Lin Group

The Lin Group has just finished its second year at UMass Chemistry. We have one postdoctoral scholar, two graduate students, five undergraduate students, and five visiting students. We are mainly interested in developing computational chemistry models that combine quantum chemistry and machine learning for applications in materials, energy, and environmental sciences.

Currently, we have three primary research directions: deciphering mechanisms of photocatalytic and electrocatalytic reactions that are significant in carbon neutrality, integrating state-of-the-art machine learning algorithms into quantum chemistry models for balanced efficiency and accuracy, and predicting electronic spectroscopy and photochemical dynamics for unconventional organic molecules for rational electronic designs. Besides pure theoretical and computational research, we also actively collaborate with computer scientists and experimental chemists in and out of UMass.



Our second academic year has been productive. We received two seed grants, including an ADVANCE Collaborative Research Seed Grant ($15,000) from UMass to develop new machine learning-based computational models for large real-life materials, and a Scialog® Team Award in Negative Emissions Science ($55,000) from Research Cooperation for Science Advancement to design unconventional electrochemical coupling of greenhouse gases. We published our very first single group research article about machine-learned density functional theory, "Stacked Ensemble Machine Learning for Range-Separation Parameters," in *J. Phys. Chem. Lett.*, and submitted our first computer science conference paper about developing a new graph neural network model. In addition to these papers, we also published three collaboration papers on diverse projects in *Proc. Natl. Acad. Sci. USA*, *ACS Energy Lett.*, and *J. Phys. Chem. Lett*. We expect the coming year to be even more productive when we are free to meet and discuss exciting problems in person.

Martin Group

While the Moderna and BioNTech/Pfizer mRNA vaccines have been a resounding success, the Martin Lab has its sights set on enabling the wealth of next generation RNA vaccines and therapeutics. The vaccine mRNAs (many 1000's of kg produced to date!) were all synthesized by T7 RNA polymerase, and for several years (starting before the pandemic), we have been on a quest to dramatically improve that synthesis by removing a long-standing road block to full implementation of mRNA therapies. Adding to our NIH support toward this effort, last Fall, the lab received a Manning-IALS award to speed development as well as a 3 year award from the Wellcome Leap R3 initiative, a DARPA-like program that aims to "increase exponentially the number of biologic products that can be designed, developed, and produced every year, reducing their costs and increasing equitable access."

Martin lab alums are a hot commodity in the RNA world. **Eddie Esposito** made the jump from the instrument company Malvern to the RNA manufacturing company Greenlight Biosciences; **Luis Ramirez** in turn, jumped from Greenlight to CATALOG DNA (which also uses our enzyme); **Elvan Cavaç** began at another RNA company, Tessera Therapeutics; and **Yasaman Gholamalipour** just started a position at Moderna after a very successful postdoc at UMass Medical.

In the lab, **Kithmie MalagodaPathiranage** has recent exciting results showing that a novel co-tethered polymerase-DNA construct can be used in a repeat batch synthesis. She has produced at least 28 rounds, with still no loss in activity — we're calling her the "energizer bunny" (but we're also looking at a robotics setup so that she doesn't wear out!). Kithmie is

collaborating with **Ruptanu Banerjee** in taking this system into a flow reactor, where we expect very long run times and very high yields! **Amin Abek** continues his work on developing sequence quality analytics – something desperately needed in this field, and will be joined by a new-to-the-lab BMB senior, **Chris Famulari**, fresh out of an internship at Moderna. A new postdoc, **Purnima Mala**, with end-user experience in T7 RNA polymerase, joined the lab in April and is off to a great start.

Undergraduate **Alex Kyranos** earned her BS in Biology this past May and will begin graduate school at UCSB in June. Together with Kithmie, she characterized the off-pathway RNA binding that leads to impurities in synthesis (presented as a poster at the RNA Therapeutics Conference in June). **Jacqueline Racine** worked with Amin and earned her BS in Biochemistry & Molecular Biology. **Josh Paine**, a rising senior in Chemistry, will continue his work with Ruptanu on post-fluidics processing. Each of them enrolled in our collaborator, Prof. Sarah Perry's, hands-on fluidics course and are excited to apply what they have learned.

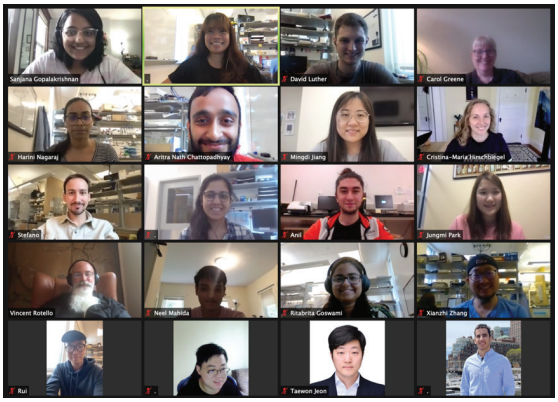
Metz Group

The Metz group is moving to lower energies – expanding our vibrational spectroscopy to the fingerprint region of the IR. Graduate student **Apakorn Phasuk** and undergraduate **Joe Gerrior** (Chemistry) studied how metal cations are solvated by acetone, and how the interaction with the metal affects the bonds in acetone by measuring the C=O and C-C-C stretches. They also observed that Al^+ catalyzes a pinacol coupling reaction between two of the acetone ligands. Graduate student **Justine Kozubal** is writing up a paper on how vanadium cluster ions V_x^+ interact with methane molecules, using vibrational spectra of the C-H stretches to determine the structures of the adducts and what they tell us about the geometries of the metal cluster ions. Graduate student **Schuyler Lockwood** is writing up results on the products, anisotropy and kinetic energy release in photodissociation of MgI^+ in the visible and UV. He and graduate student **Gaurav Singh** are improving the capabilities of our photofragment imaging instrument. The NSF has funded a grant to extend our studies to look at reaction kinetics of sequential reactions of metal and metal cluster ions with methane and to use vibrational spectroscopy to characterize the products, as well as to use photofragment imaging to measure covalent bond strengths in metal carbenes and methides. Several group members will be presenting their results at the Molecular Interactions and Dynamics Gordon Conference, for which Rick is the vice-Chair.

We had a recent visit from alum **Affawn Ashraf** (Intel). We love hearing from group alumni — please let us know what you're up to!

Rotello Group

Vince is looking forward to getting back on the road—this is the first time he's stayed home for over a year since he arrived at UMass in 1993, and now it's two years(!). He has been presenting, however, with four talks at PacificChem in virtual Hawaii (boo!), one in Pakistan, and a few others scattered around the US. Just this April, he was identified by Research.com as among the top scientists for two fields: Chemistry (#396 world ranking; #190 in the US) and Materials Science (#281 world ranking; #125 in the US)! Additionally, Vince has been named a Clarivate "Highly Cited" researcher again in 2021. The publication total is ticking up, with the current count at 625. The group has its fingers crossed for the renewal of their antimicrobial grant—$1.9M, and it scored in the top 2%.



Xianzhi Zhang won the William E. McEwen scholarship award for Outstanding Oral Presentation (Second Place) during ResearchFest 2021. He was also awarded the Marvin D. Rausch Fellowship for outstanding research in the area of Organic or Inorganic Chemistry! **Jessa Marie Makabenta** won the People's Choice Award during the 2022 UMass Three Minute Thesis (3MT) Finals competition.

We have had a strong influx of new faces including **Junwhee Yang** and **Muhammad Aamir Hassan** who have officially joined our group as graduate students. We also welcomed **Dr. Victor Louis Adam Lehot** as a postdoctoral fellow and **Prof. Mehmet Gokhan Caglayan** joined as a visiting Fulbright Scholar. Welcome to the group!

For up-to-date news, please check out http://www.umass.edu/rotellogroup/ or see what's up on our social media accounts: Facebook https://www.facebook.com/rotellogroup and Twitter https://twitter.com/RotelloGroup.

This will hopefully be the last virtual group picture. Everyone is looking forward to strike a pose for an in-person group photo!

Skouta Group

The Skouta lab is excited to continue advancing our medicinal and chemical biology research projects focusing on small molecules probing diseases. The lab is participating in the department and CNS mission of educating the next generation of scientists from all backgrounds including URM students.

Professor Skouta was honored and touched by students' recognition/nomination for the third time in a row as one of the finalists of the 2022 Distinguished Teaching Award (DTA) at UMass. The Skouta team published two manuscripts: "FDA-Approved Oximes and Their Significance in Medicinal Chemistry" and "The Selenoprotein Glutathione Peroxidase 4: From Molecular Mechanisms to Novel Therapeutic Opportunities."

This year we said goodbye to undergraduates **Kamari Weaver** (a 2021 LSAMP recipient), **Jasmin Gray** (a 2020 LSAMP recipient) and **Ellen Kernan** (a 2021 Lee Sip Recipient). Kamari was the first author of our recently published work on "The Selenoprotein Glutathione Peroxidase 4: From Molecular Mechanisms to Novel Therapeutic Opportunities". Kamari

received a degree in biochemistry and will be pursing an MD-PhD program. Ellen Kernan successfully secured an industrial job at Microbiotix Worcester after graduating with a BS in chemistry. Jasmine received her BS in biochemistry and is currently working at the Biomarker Research and Clinical Trials Laboratory, Brigham and Women's Hospital in the Petr Jarolim Lab as a research associate.

This year we welcomed undergraduate chemistry major researchers **Liam Murphy**, **Brennan McAvoy,** and **Patrick Doucette**, as well as **David Figueredo Picon** (Biochemistry) and **Gabe Zeinoun** (Biology). Liam Murphy was recognized at the 2022 Departmental Senior and Awards Dinner, receiving the Mahoney Undergraduate Research Award to perform research in the Skouta lab. Currently Liam is a process engineering/chemistry intern with Impact Nano at their Research and Development lab in Devens, MA. His main project this summer will be working on the synthesis of an organometallic tin compound for use in the chip manufacturing process using the principles of green chemistry. Brennan is working in LAL (Limulus amebocyte lysate) production for Associates of Cape Cod in Falmouth, MA. LAL is used to test for endotoxins and gram negative bacteria to ensure sterility. Gabe was a Lee SIP (William Lee Science Impact Program) recipient to perform research in the lab this summer.

Thayumanavan Group

The Thayumanavan group enjoyed another productive year in 2022.

Graduate students update: **Prachi Gupta** and **Yasin Alp** joined the group early in 2022. For our current graduate students, we congratulate **Jingyi Qiu** for receiving the Inspiration Award for Neuroscience and Technology from the Neuroscience and Behavior program at UMass Amherst.

We also congratulate our Alumni, **Jingjing Gao**, for being acknowledged as a 2022 Young Investigator and Future Faculty Scholar. Congratulations to our undergraduate student, **Amelia Isabelle**, for receiving the 2022 Positron Award from UMass Chemistry.

Hongxu Liu, after finishing his PhD, is now a postdoctoral associate at the University of Texas at Austin. **Khushboo Singh** finished her PhD in August 2021 and has taken a job as Research Fellow at Vertex Pharmaceuticals in San Diego, California. Dr. **Thameez Mohammed Koyasseril Yehiya** joined an ever-growing cadre of Intel employees in Portland, Oregon. He was a Post-Doctoral Research Associate in the Siegrist Group in Microbiology here at UMass, after finishing his PhD in the group.

Undergraduate students update: **Joseph Matte**, **Rahul Sharma** and **Maxwell Bowen** all graduated. Rahul is pursuing his MS in Biomedical Engineering at University of Pennsylvania. **Ramita Kommuru**, **Logan McCarthy**, **Liliana Florino**, and **Amelia Isabelle** joined our group for undergraduate research recently.

Thai has been named head of the Biomedical Engineering Department (BME) in the College of Engineering. He served as the interim department head for biomedical engineering since January 2021 before being named for the permanent position in January of 2022.

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

Thompson Group

We are happy to welcome to the lab Chemistry graduate student **Isabella (Bella) Jankowski**, who joined the group in December. Congratulations to graduate student **Jessica Allen** who was awarded a CBI Traineeship in September 2021, to undergraduate **Sarah Tobia** who received the Tarselli Family Research Award in May 2022, and to **Lynmarie** who was selected as a AAAS Fellow, and also received the UMass CNS

Outstanding Service and Engagement Award.

Thomas Tran, Bella Jankowski, Jessica Allen, and Katie Wahlbeck

We have very much enjoyed being back together in person this year, including some fun outings with the 8th floor labs, canoeing in July 2021, and "sugar shacking" in March 2022. In-person conferences resumed for us with the Biophysical Society Meeting in February 2022, which both Lynmarie and Jessica Allen attended, and several more conference trips are planned for this summer. After a two-year hiatus, we finally had a Drug Design field trip in April 2022, to Roivant Sciences in Boston, and all of our lab's graduate students attended.

Vachet Group

A full year back in the lab in person was great for the entire group. Many students leveraged new computational skills that they had learned during the lab shutdown to enhance their research. Whether it was learning Python to streamline data analysis and analyze mass spectrometry imaging data, or applying molecular dynamics simulations to understand protein structure, Vachet group members emerged from the pandemic shutdown with some great science. We

continue NIH-funded work on protein amyloid formation and NSF-funded work on new mass spectrometry imaging methods. In the past year, the group published seven peer-reviewed papers on topics that ranged from mass spectrometry imaging of nanomaterial drug delivery systems, to protein structure prediction with mass spectrometry, and computational methods to new methods for mapping epitopes in antibody-antigen complexes.

In group news, we said farewell to three PhD students. **Laura Castellanos** defended her PhD in August after developing new mass spectrometry imaging data analysis methods that were a new research thrust in the group. Laura is now applying her mass spectrometry skills at Tessera Therapeutics in Cambridge, MA. Ten days after Laura's PhD defense, **Catherine Tremblay** successfully defended her thesis work on the structural analysis of protein therapeutics using mass spectrometry. Soon after, Catherine headed to Waters Corporation where she now works as an applications chemist. **Xiao Pan** was the third PhD student to finish when she presented her studies on protein higher-order structural analysis by covalent labeling mass spectrometry. Xiao is now a postdoc at Genentech in California.

Four Chemistry majors who did research in the group also finished up in May. They included **Zach Danaceau**, **Sam Regan**, **Adam Elmasri**, and **Josh Lauterbach**. Zach, Sam, and Adam are all headed off to graduate school in Chemistry, while Josh has started working at Matterworks in Cambridge, MA.

We welcomed four new graduate students into the group: **Trisha Brady**, **Kanitin 'Minion' Khamnong**, **Michael Moore**, and **Vanessa Stahl**. Trisha was an undergraduate student at the University of New Haven where she did her studies with group alumna **Alyssa Marsico** (PhD 2016). Trisha is jointly advised with Prof. Jeanne Hardy, and she will be using native mass spectrometry methods to study caspase complexes. Minion came from Chulalongkorn University in Thailand, where group alumni **Nadnudda 'Tan' Rodthongkum** (PhD 2011) and **Patanachai 'Kong' Limpikirati** (PhD 2020) are currently faculty members. Minion will be developing methods to characterize membrane protein binding in cells. Michael received his undergraduate degree at Tufts University before working for a few years as a laboratory technician. He will be using ion mobility mass spectrometry to study protein amyloid formation. Finally, Vanessa did undergraduate work at Boston University before coming to UMass as an MCB student. She will also be working with Prof. Jennifer Rauch in the BMB Department, studying the structure and interactions of the protein Tau, which is important in Alzheimer's disease.

In alumni news. . . **Matthew Miller** (PhD 2006) started a new job as Global Product Leader at CSL Behring; **Bo Yan** (PhD 2014) and his wife Ting welcomed their second son in February; **Meizhe Wang** (PhD 2019) had a son, Levi, in June of 2021; and **Ben Ditrolio** (BS 2008) is now working on his Master's degree in Oceanography at Dalhousie University in Halifax, Nova Scotia.

Venkataraman Group

The Advanced Laboratory for Iontronic, Electronic, and Nanomaterials (ALIEN) group, aka DV group, had a great 2021-2022 academic year. **Emily Smith** received the Marvin D. Rausch Lectureship award for outstanding oral presentation in our annual ResearchFest. **Michael Lu-Díaz** and **Subhayan Samanta** received William E. McEwen Fellowship Awards for outstanding poster. Michael was also awarded

the Donald Kuhn Graduate Fellowship and was one of three students selected for the university's Scientist Mentoring and Diversity Program. This program provides "Career development coaching, one year of personalized career mentoring and guidance from an industry leader, networking opportunities and financial support to attend a major industry conference." **Garrett Miskell** received the ACS Award for Inorganic Chemistry.

We welcomed **Mitchell Willsey** to our group as a graduate student. He comes to UMass from Bates College and his research is focused on developing efficient and air-stable n-type dopants for polymer semiconductors. We also welcomed **Simon Harrity**, an undergraduate researcher interested in synthetic chemistry. **Armaan Munsiff**, an undergraduate pursuing an Economics Major, joined the group in April to study the supply chain and equity issues associated with perovskite solar cells. **Hamza Javaid** and Emily Smith graduated with their doctoral degrees. Hamza is currently a TD Module and Integration Yield Engineer at Intel in San Jose, CA. Emily will be joining the Naval Research Laboratory in Washington, DC. Garrett Miskell graduated with a BS (honors) in Chemistry and will join the radiopharmaceutical facility at the Mass General Hospital in Boston. **Priya Srivastava** returned to IIT Roorkee in India after completing her Fulbright Fellowship. She defended her doctoral dissertation and is now a Research Associate at IISER in Thiruvananthapuram, India.

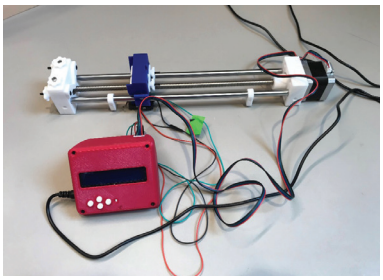
ALIENs: (l-r) Garrett Miskell, Mitchell Willsey, Michal Lu-Diaz, Simon Harrity, DV, Eric Ostrander, Emily Smith, Zhaojie Zhang, Subhayan Samanta and Armaan Munsiff

From the alumni side, **Prof. G. Nagarjuna** received tenure and was promoted to Associate Professor at Georgetown University. He also received a 2021 ASC PMSE Young Investigator Fellowship. **Prof. Monojit Bag** received tenure and was promoted to Associate Professor at IIT Roorkee. **Dr. Sravan Surampudi**, who is a lecturer in Chemistry, received the Chemistry Department Distinguished Undergraduate Instructor Award in Honor of Earl J. McWhorter and George R. Richason Jr. He was also a member of the CNS Lecturer's Council, which won the inaugural Equitable Practices in Collaboration and Shared-Decision-Making (EPiC-SD) Award from the UMass ADVANCE program. DV also had a chance to meet **Dr. Seung Pyo Jeung**, now a Research Scientist at CooperVision in CA, when DV was on a visit to Merced. Seung Pyo, Hamza and DV met at Tracy, which is midway between San Jose and Merced. **Sam Knight**, who is now a graduate student at the University of Chicago has joined Prof. Andrei Tokmakoff's group to study hydrophobic effects in water using 2D-IR spectroscopy. **Matthew 'Donnie' Rollings** in an NSF Fellow and working with Prof. Felix Fischer at UC Berkeley on 1D and 2D based graphene spin systems. DV is proud of your achievements and loves to hear from all of you. So, drop a line when you can to dv@umass.edu. For group updates and news, visit us on the web at thedvgroup.com and follow us on twitter @dvgroupumass or Instagram at dvgroup_umass.

Dr. Sravan Surampudi receiving his award from Dr. Xueying (Sharon) Qin

DV met Dr. Seung Pyo Jeung and Dr. Hamza Javaid in Tracy, CA

Research wise, the group's focus is now organic and hybrid semiconductors. We have started to unravel the role of dopants in organic semiconductors and the role of interfaces on the stability of halide perovskites. We also updated the NREL Best PV research cell efficiencies chart as an interactive Tableau viz. You can check out this interactive chart at https://dvgroup.umasscreate.net/pv-research-cell-efficiencies/. You can now download the charge as an image file, PPT or PDF, and you can choose the sections of the graph that are of interest to you. DV is also currently serving as Chair of the Organizing Committee for the NSF 2026: Workshops to Identify Priorities and Research Needs for an Equitable Energy Transition. The goal of these workshops, funded by the National Science Foundation, is to integrate diverse perspectives across disciplines and sectors in the US energy system and identify specific research priorities at the intersection of energy, technology, and social justice. This has been eye-opening as DV is learning a lot about inequities associated with several energy technologies. You can also learn about some of these issues at https://nsf2026.umasscreate.net



A syringe pump built by Zhaojie Zhang using 3D printed parts

Finally, in the last GG note, I had mentioned that we have a new toy, a 3D printer, thanks to a grant that Emily received from UMass. This printer has become an invaluable tool in the group for 3D printing things in the lab. The latest is an ultrafast syringe pump built by Zhaojie for injecting solvents on perovskite films. Even the red control box casing was 3D printed!

Walsh Group

The 2021–2022 academic year was a big one for undergraduate awards in the Walsh Lab. **Laura Casey** (senior in the Honor's College) was recognized for her dedicated work as a general chemistry TA with an honorable mention for the "Top Gun" Award. **Wyatt Mitchell** (rising junior) was awarded the Roger G. Bates Fund, which will allow him to continue his high-pressure synthesis research in our lab over the summer. **Zeynep Alptekin** (rising senior), was named a recipient of the prestigious Barry M. Goldwater Scholarship as well as the UMass Rising Researcher Award 2022. In addition, her poster presentation detailing her work on the high-pressure synthesis of cobalt cementite earned her the Uche Anyanwu Memorial Award for outstanding poster. We are very proud of all of them! Graduate student **Paul Marshall** published his work on cobalt cementite in *Chemistry of Materials*, which was also featured on the front cover. Graduate students **Nick Manganaro, Scott Thiel,** and **Kimberly Bolduc** were all recognized as Chemistry Ambassadors by the UMass Chemistry Department Recruitment Committee, and will visit their alma mater institutions in the fall. In the coming summer months, the Walsh Group will be writing up the next round of papers, carrying out even more experiments at the Advanced Photon Source, and preparing to present at conferences to share some of our exciting recent results with the broader chemistry community.

You Group

This past year we graduated the first batch of PhD students from the You Lab! **Qikun Yu** is now a Scientist at PTC Therapeutics. **Yousef Bagheri** joined Prof. Sarah Veatch's lab at the University of Michigan as a postdoctoral fellow. **Puspam Keshri** became a Scientist at Laronde, and **Rigumula Wu** joined Genentech. We also had five undergraduate researchers, **Jikun Wang**, **Saoirse Connolly**, **Jahn Pothier, Simon Kangoun**, and **Sidrat Siddiqui**, who graduated last year. We will miss all of you! On the other side, we also welcomed a new research

fellow, **Dr. Yuanchang Liu**, and four new undergraduate researchers, **Sarthak Srivastava**, **Michelle Moskvitch**, **Kevin Alexander**, and **Anastasiya Kaltashova**.

Prof. Mingxu You submitted his tenure package, which has now been recommended by the Chancellor and Provost in favor of tenure with promotion to Associate Professor. In addition, he received a prestigious Burlew Award from the Connecticut Valley Section of the American Chemical Society. Prof. You is now an associate editor of *Frontiers in Chemistry,* while continuing to serve on the editorial board of *Membranes*, *Biosensors*, and *PeerJ Analytical Chemistry*. Our lab members have also obtained several awards and achievements. **Zhining Sun** received a Paul Hatheway Terry Scholarship in recognition of his research and academic standing. **Ru Zheng** was awarded a two-year Chemistry-Biology Interface Fellowship. During ResearchFest 2021, **Rigumula Wu** was awarded a William E. McEwen Scholarship Fund Award for her oral presentation, and **Ru Zheng** was a first-place winner of the Marvin D. Rausch Scholarship Award for outstanding poster presentation. **Ahsan Ausaf Ali** and Ru Zheng have passed their original research proposal defense and become PhD candidates. **Qian Tian** is taking a 3-month summer internship at Dyne Therapeutics. Ahsan Ausaf Ali will take an internship at Agios Pharmaceuticals.

We have continued our research in developing next-generation RNA-based biosensors for cellular imaging and regulation, as well as cell membrane-modified DNA probes to measure mechanical forces at cell-cell junctions. We have published one book chapter and seven manuscripts this year in these directions. We are looking forward to an even more fruitful year. For more information, please visit our website: https://elements.chem.umass.edu/youlab/ or Twitter: https://twitter.com/UMass_YouLab

The department celebrated Prof. Bret Jackson's retirement last fall. Current and retired faculty and a few spouses gathered for a photo. Left to right: James Walsh, Mingxu You, Janiece Leach, Rick Metz, Peter Lillya, Craig Martin, Scott Auerbach, Nate Schnarr, DV Venkataraman, Jeanne Hardy, Joe DuChene, Bret Jackson, Paul Lahti, Margaret Rakas, Jianhan Chen, Ed Voightman, Min Chen, Mike Maroney, Richard Vachet, Vince Rotello, Julian Tyson, Igor Kaltashov, and Holly Davis

Seminar by Joseph DuChene, Seminar Chair

The Chemistry Department was very excited to finally return to in-person seminars this past year! We were honored to host so many talented scientists and distinguished speakers for the 2021-2022 UMass Amherst Department of Chemistry seminar series.

In October of 2021, **Professor Zhenan Bao** from Stanford University presented the Stein-Covestro Honorary Seminar in Polymer Chemistry. Professor Bao is the K. K. Lee Professor of Chemical Engineering, with courtesy appointments in both Chemistry and Materials Science & Engineering. She is an internationally recognized leader in polymer chemistry who has founded several companies and serves as the Faculty Director of the Stanford Wearable Electronics Initiate (eWEAR). Professor Bao is also a Fellow of the National Academy of Engineering, the National Academy of Inventors, and the American Academy of Arts and Sciences. Professor Bao gave a very exciting presentation discussing her group's recent progress towards the development of skin-inspired organic electronics for the eventual realization of stretchable, self-healable, and biodegradable conductive or semiconducting materials with applications ranging from energy storage to wearable electronics.

Prof. Zhenan Bao

In March of 2022, the Annual 5-College Lecture Series in Chemistry resumed after a two-year hiatus due to the global pandemic. **Professor Richmond Sarpong** from the University of California Berkeley was the honory speaker. Professor Sarpong's work is focused on the total synthesis of biologically active natural products as a platform for developing new synthetic methods and strategies. He shared his unique perspective on how his group approaches challenging problems in organic synthesis with a very engaging seminar, entitled "Break-It-To-Make-It Strategies for Complex Molecule Synthesis." Everyone enjoyed Professor Sarpong's presentation, and we were all very happy to have the Annual 5-College Lecture Series in Chemistry held in-person once again!

Prof. Richmond Sarpong

Prof. Gregory Robinson

In April of 2022, **Professor Gregory Robinson**, the UGA Foundation Professor of Chemistry at the University of Georgia, gave the annual Marvin D. Rausch Lecture in Organometallic Chemistry. Professor Robinson is a Fellow of the Royal Society of Chemistry and is a member of the National Academy of Sciences. His research focuses on understanding the chemistry of the main group elements with particular emphasis on the synthesis of organometallic compounds with unusual bonding, such as the first compound containing a gallium-gallium triple bond. Professor Robinson gave a very entertaining presentation recounting his group's successful synthesis of the first compound containing a boron-boron double bond, along with several other new directions, such as the stabilization of elusive main group oxides of silicon and phosphorus.

Prof. Laura Kiessling

Professor Laura Kiessling, the Novartis Professor of Chemistry at MIT, had to postpone giving the William E. Mahoney Annual Lecture due to COVID-19. Her research interests have led to advancements in the cell surface recognition processes, in particular protein-glycan interactions, and we look forward to hosting her talk "Glycan Polymers in Health and Disease" this fall.

We also virtually hosted many luminaries in the field of chemistry, including **Prof. Ashkan Salamat** (University of Nevada, Las Vegas), **Prof. Nick Stephanopolous** (Arizona State University), **Prof. Chengxian Lin** (Yale University), **Prof. Nagarjuna Gavvalapalli** (Georgetown University), **Prof. Jinjun Liu** (University of Louisville), **Prof. Eman Akam** (Harvard University), **Prof. Renee Frontiera** (University of Minnesota), **Prof. Stuart Lindsay** (Arizona State University), **Prof. Jia Niu** (Boston College), **Prof. Arthur Tinoco** (University of Puerto Rico), **Prof. Fikile Brushett** (MIT), **Prof. Wenjie Dou** (Westlake University), **Prof. Aleksei Aksimentiev** (University of Illinois Urbana-Champaign), **Prof. Thao Tran** (Clemson University), **Prof. Ishac Nazy** (McMaster University), and **Prof. Crina Nimigean** (Cornell University). The variety of such great scientific speakers was truly inspiring, and we look forward to another exciting seminar series next year!

The Chemistry Department is very grateful for the generous contributions of our alumni and corporate sponsors, who make the success of the seminar program possible. More information about upcoming seminars and events can be found at www.chem.umass.edu/events- seminars/.

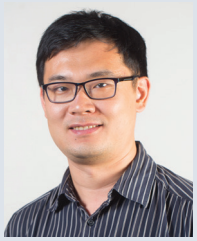
faculty
Promotions

Assistant Professors **Michelle Farkas** and **Mingxu You** have been recommended for tenure and promotion to Associate Professor by the Provost and Board of Trustees. Their promotions will take effect September 1, 2022. Associate Professor **Eric Strieter**'s promotion to Full Professor has been approved by the Provost and Chancellor. It will also take effect September 1.

Michelle Farkas

Prof. Farkas started as an Assistant Professor in the Chemistry department in 2013. Her interdisciplinary research program studies circadian rhythms and macrophages and their connections to cancer. Prof. Farkas has developed bioluminescent tools to monitor the real-time activity of circadian clock genes in cells, and chemicals to perturb the period and stability of the circadian cycles. This combination of tools has allowed her to study the mechanisms that connect circadian rhythms and cancer progression. Prof. Farkas' second major research direction is on macrophages, key components of the immune system's response to tumors. They can switch between immune-suppressing and immune-stimulating states, which has implications for cancer metastasis. Prof. Farkas has developed tools to monitor the macrophage phenotype, assessing how they are altered and modulated by different conditions and treatments. As macrophages can also be used to target cancer cells, Prof. Farkas and her lab have been developing chemically modified macrophages as delivery vehicles for imaging and therapeutic agents, along with studying the impacts of the modifications on cellular characteristics.

Mingxu You



Prof. You started as an Assistant Professor in the Chemistry department in 2016. He develops sensors based on DNA and RNA and uses them to a) image and measure molecules in living cells, b) measure forces between cells and c) image lipid domains in cell membranes. These tools have been used by the You group and many collaborators to understand cell function and mis-function. The sensors for molecules use RNA aptamers to selectively bind to a target analyte and to a fluorescent dye. When both are present, the sensor will fluoresce when illuminated. This enables him to measure—in a living cell—how much of a molecule is present and where it is located. He has used the aptamer-based sensors to detect a wide range of small molecules including metal ions, antibiotics, large proteins and RNAs. A second project develops fluorescent hairpin-shaped DNA-based probes to measure forces between cells, with both spatial and temporal resolution. Mechanical forces between cells are important to cell development, morphogenesis, and cancer metastasis. In a third major project, Prof. You has developed new tools to image lipid-lipid and protein-protein interactions and has used them to study the dynamics of lipid domains in cell membranes. Because these lipid domains are not uniformly distributed and their distribution changes with time, they have proven to be very challenging to study.

Eric Strieter

Prof. Strieter joined the Chemistry department as an Assistant Professor in 2016, moving his lab from the University of Wisconsin. He was promoted to Associate Professor with tenure in 2018. His research uses a combination of chemical tools, biophysical methods, and cell biology to elucidate how the small protein ubiquitin controls the dynamics of biochemical pathways to maintain normal cellular function. One or several ubiquitins can be added to a target protein and they can link together at different positions, forming chains that can be linear or branched. The pattern of ubiquitins on a protein controls where it will go in a cell, affects how it functions, and if it will be digested by the proteasome. Addition and removal of ubiquitin (ubiqitination and deubiquitination) comprises an intricate signaling pathway and is an important mechanism to regulate protein function and maintain protein homeostasis. Prof. Strieter's research seeks to understand how this system works — how (and where) ubiquitins are added and removed and how the enzymes that carry out these reactions recognize specific ubiquitin chain topologies and react with them. Prof. Strieter has developed chemical tools to determine the biochemical properties of different ubiquitin modifications, and to determine and quantify their presence in cells. Building on this work, he has used these tools to decrypt the "ubiquitin code" and understand and manipulate the mechanisms by which protein degradation is regulated.

31st annual

ResearchFest

The 31st annual research symposium, ResearchFest, introduced first year students to our program, faculty, staff, and fellow students. The department held an in-person event this year, switching back from the virtual remote format held in 2020.

The keynote address was given by **LT Elih M. Velazquez-Delgado**, PhD'12 (Hardy Group), Department Head, Scientific Research at Armed Forces Radio Research Institute, Uniformed Services University of Health Sciences.

The three alumni Career Panelists were **Mary Kate Donais** PhD '91 (Uden Group), **Derek McPherson** PhD '18 (Hardy Group), and **Sean Crowe** PhD'18 (Strieter Group). Donais is a fellow of the SAS and the Royal Society of Chemistry, and is focused on spectroscopy and portable instrumentation, especially applications in the fields of archaeology and cultural heritage. McPherson is a Senior Investigator at Roivant Discovery and has participated in a number of high profile drug discovery campaigns working actively as a biophysics specialist purifying and characterizing proteins, developing assays, as well as a number of activities around protein structure including crystallography and hydrogen deuterium exchange mass spec. Crowe is a Research Scientist in the Bioproduct Research and Development group at Eli Lilly and Company.

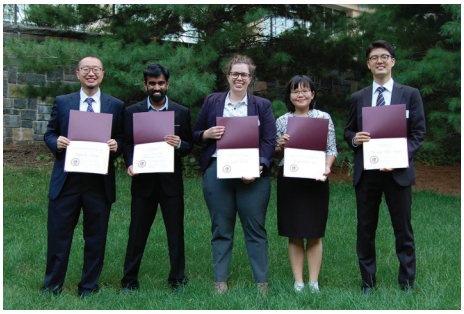
The Marvin D. Rausch Scholarship Award for Outstanding Oral Presentation was awarded to **Emily Smith** (DV group) for her talk "The Curious Case of Copper Iodide in Perovskite Solar Cells." **Kwang-Won Park** (Andrew group) received the Paul Hatheway Terry Endowment Award as first-runner up for his talk titled "Enhanced Emission of Molecular Thin Films via Seed-induced Crystallization and Their Applications for Organic Solar Cells and Light Emitting Diodes." **Xianzhi Zhang** (Rotello group) won the William E. McEwen Scholarship Fund Award as a joint first-runner up for his talk "Transition Metal Catalyst-nanoparticle nanozymes for anticancer therapeutics." **Sujeewa Sampath Lellupitiyage Don** (Farkas group) won the Paul Hatheway Terry Endowment Award as a joint second-runner up for his talk "Circadian Rhythms Exist in Low Malignancy MCF7 Breast Cancer Cells and Nobiletin Rescues Oscillations in Triple-Negative MDA-MB-231 Cells." **Rigumula Wu** (You group) won the William E. McEwen Scholarship Fund Award as a joint second runner up for her talk "Genetically Encoded RNA-based Sensors for Quantitative and Multiplex Imaging in Living Cells."

The Marvin D. Rausch Scholarship Award for Outstanding Poster Presentation was awarded to **Ru Zheng** (You group).

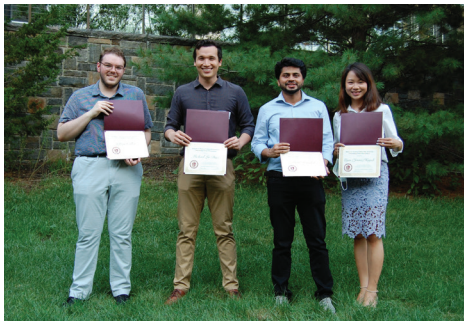
Seven students received the William E. McEwen Award for Outstanding Posters. Securing first position were **Fanjun Li** (M. Chen group) and **Uyen (Jennie) Huynh** (Thayumanavan group). **Pintu Kanjilal** (Thayumanavan Group) received second position, **Michael Lu-Díaz** (Venkataraman Group) and **Nicholas Hight-Huf** (Barnes Group) earned third position, and **Jeffrey Cullen** (Farkas Group) and **Dheeraj Agrohia** (Vachet Group) were voted People's Choice.

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, and alumni. We also thank the following vendors who came to show us what their companies had to offer: Beckman Coulter, ChemGlass Life Sciences, Corning, JH Technologies, Max Analytical Technologies, Millipore Sigma, Takara, Thermo Fisher Scientific, and Wilkem Scientific.

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



Talk Winners (left to right): Xianzhi Zhang, Sujeewa Sampath Lellupitiyage Don, Emily Smith, Rigumula Wu, and Kwang Won Park



Poster Winners: Jeffrey Cullen, Michael Lu-Diaz, Pintu Kanjilal, and Uyen (Jennie) Huynh

Incoming Fall 2021 Graduate Students: Michael Moore, Isabella Jankowski, Mitchell Willsey, Prachi Gupta, Junwhee Yang, Lauren McDonald, Kanitin Khamnong, and Trisha Brady. Not pictured: Yasin Alp, Kevin Cheung, and Muhammad Aamir Hassan

ResearchFest poster session in the Integrated Sciences Building (ISB) atrium

PhD defenses

September 2021 - July 2022

Linden Kohler Allison, *"An Exploration of the Thermoelectric, Thermoresistive, and Hygroresistive Properties and Applications of Vapor Printed PEDOT-Cl,"* Trisha Andrew

Jillian Denhardt, *"Formation Of Doped Semiconductor Nanocrystals From Doped Molecular Clusters,"* Kevin Kittilstved

Sujeewa Sampath Lellupitiyage Don, *"Tracking And Modulating Circadian Rhythms In Cell Culture Models,"* Michelle Farkas

Sanjana Gopalakrishnan, *"Biomedical Applications of Protein Films and Polymeric Nanomaterials,"* Vincent Rotello

Hamza Javaid, *"Tailoring Interfaces and Composition for Stable and Efficient Perovskite Solar Cells,"* D. Venkataraman

Bishnu Prasad Joshi, *"Surface Modification Of Macrophages And Stem Cells: Effects Of Biocompatable Conjugates On Cell Behavior,"* Michelle Farkas

Puspam Keshri, *"Quantitative imaging of tensile forces at cell-cell junction with DNA-based probes,"* Mingxu You

Fanjun Li, *"Investigation of kinase conformational dynamics and analytes detection with protein nanopore,"* Min Chen

Kithmie H MalagodaPathiranage, *"Mechanism-driven approaches and novel constructs for high purity RNA synthesis,"* Craig Martin

Arash Manafirad, *"Manipulating the Properties of Light-Responsive Active Lipid Bilayer Membranes: Measuring Mechanics and Probing Mechanisms,"* Anthony Dinsmore (Physics)

Babgen Manookian, *"Molecular Vibrations and Shape-Selectivity: A Computational Model of Biofuel Precursors in Zeolites,"* Scott Auerbach

Xiao Pan, *"Deciphering Protein Higher-Order Structure and Interactions via Diethylpyrocarbonate Labeling-Mass Spectrometry,"* Richard Vachet

Kwang-Won Park, *"Vapor Deposition Strategies for Tuning Surface and Interface Chemistry for Optoelectronics and Biosensors,"* Trisha Andrew

Emily C. Smith, *"Elucidating the Function of Ions in Hybrid Perovskite Photovoltaics,"* D. Venkataraman

Ishankumar V Soni,*"Investigating Structures and Functions of Apoptotic Caspases,"* Jeanne Hardy

Rigumula Wu, *"Multi-colored fluorogenic RNA sensors for the quantification and multiplexed imaging of small-molecule levels in living cells,"* Mingxu You

Yang Yang, *"Studies of Heterogeneous Macromolecules using Novel ESI Mass Spectrometry Based Approaches,"* Igor Kaltashov

Chemistry Department Ambassador Program

Spring 2022 welcomed the first awardees of the Chemistry Department Ambassador program, which provides support for graduate students to visit their alma mater institution to deliver special seminars. The ambassadors will present on not only their research accomplishments, but also on their experiences as a chemistry graduate student at UMass Amherst. The program aims to strengthen our ties with other departments by showcasing the excellence achieved by the students in our program, and will hopefully inspire the next generation to follow in their footsteps. The inaugural awardees are **Kimberly Bolduc** (Union College, NY), **Gaurav Mitra** (Modern College of Arts, Science and Commerce, Pune, India), **Nathanael Kuzio** (Bates College, ME), **Scott Thiel** (Rensselaer Polytechnic Institute, NY), and **Nick Manganaro** (University of New Haven, CT).

2022
Undergraduate Awards

The department hosted an in-person Undergraduate Awards Ceremony on April 28th at the Campus Center. Students and their families were joined by faculty, staff, donors, and Dean Serio to recognize the hard work and dedication of our students and their exceptional achievements.

Donors were also invited to talk about their awards, awardees had the opportunity to say a few words of thanks, and research advisors introduced the research award winners from their groups.

The awards are made 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.

Research group noted in parenthesis.

Academic Awards

American Chemical Society (ACS) Hach Scholarships
Jenna Lutz and Kael Pelletier

ACS Undergraduate Award in Analytical Chemistry
Owen Doyle (DuChene)

Edward Shapiro Fund
Erika Brown, Sheehan Choudhury, Nicholas Dix, Fiona McEvoy and Megan Yee

Jay A. Pirog Scholarship
Hallee Yoder

John A. Chandler Memorial Scholarship
Hanwen Chen (Rotello) and Alanna Mahar (Hardy)

Michael Bruno Scholarship
Brandon Tsang

Robert Maxwell Williams Memorial Scholarship
Olivia Arnold, John Burton, and Henry Raughley

Royal Society of Chemistry Certificate of Excellence
Ethan Goulart (Hardy)

Thomas R. "Casey" Stengle Scholarship
Snayha Bhuiyan (M. Chen) and Terry Nguyen (Rotello)

Research Awards

ACS Undergraduate Award in Inorganic Chemistry
Garrett Miskell (DV)

ACS Undergraduate Award in Organic Chemistry
Ethan Goulart (Hardy)

ACS Undergraduate Award in Physical Chemistry
Timothy Yesepkin (Auerbach)

Chemistry Undergraduate Research Fund
Erika Brown (DuChene)

Dr. Uche Anyanwu Memorial Fund
Zeynep Alptekin (Walsh), Ethan Goulart (Hardy) and Bao Le (Farkas)

J.F.B. Fund for Undergraduate Research
Kevin Alexander (You)

Mahoney Undergraduate Summer Research Award
Bao Le (Farkas) and Liam Murphy (Skouta)

Mr. Tompkins Award
Ethan Goulart (Hardy) and Bao Le (Farkas)

Oliver Zajicek Memorial Scholarship Award
Zachary Danaceau (Vachet) and Jikun Wang (You)

Professor Jack Ragle Endowed Fund in Chemistry
Pranav Viswanathan (Muthukumar)

Roger G. Bates Chemistry Fund
Wyatt Mitchell (Walsh)

Sir Harold W. Kroto and Steve F.A. Acquah GEOSET Award
Grace Rogers (Auerbach)

Tarselli Family Research Award
Sophie Spielberger (Farkas), and Sarah Tobia (Thompson) and Pranav Viswanathan (Muthukumar)

Departmental Awards

ACS-Connecticut Valley Section Student Award
Ethan Goulart (Hardy)

American Chemical Society Membership Awards
Ethan Goulart (Hardy) and Nhu Nguyen Anh Ngo (Crosby)

American Institute of Chemists Award
Nhu Nguyen Anh Ngo (Crosby)

Departmental Recognition Award
Ethan Goulart (Hardy) and Nhu Nguyen Anh Ngo (Crosby)

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

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

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

Positron Award
Amelia Isabelle (Thai)

Richard W. Fessenden Award
Owen Kuklinski (Knapp)

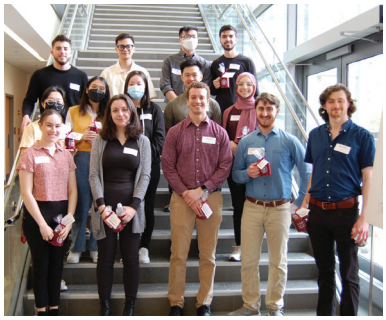
Senior Class Award
Ethan Goulart (Hardy)

undergraduate

Poster Session

Chemistry's 2022 Undergraduate Research Poster Session was held on April 8th in the Intergrated Sciences Building (ISB) Atrium. Fourteen students presented their posters to faculty and students.

The Dr. Uche Anyanwu Memorial Fund recognizes the top three research posters presented by students working in chemistry labs. The fund was established by Dr. Ucheoma O. Akobundu to honor her late husband, Dr. Anyanwu, who was the first member of the D. Venkataraman (DV) group, earning his PhD in 2005.

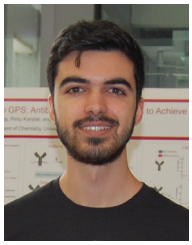


The awardees were senior Ethan Goulart, and rising seniors Zeynep Alptekin and Bao Le.

Exploring the Cobalt-Carbide System at High Pressures Zeynep Alptekin '23

Materials discovery is critical to technological advancements, from improving the efficiency of renewable energy harvesting with cheaper and stronger permanent magnets, to building next-generation hypersonic air and spacecrafts. In the Walsh lab, my project is on the cobalt–carbon system, as the withdrawal from lanthanoid elements such as neodymium and dysprosium is critical for the longevity of rare-earth natural resources on the planet. However, the cobalt–carbon system does not have any thermodynamically stable compounds at atmospheric pressures. We used Ab Initio Random Structure Searching (AIRSS) coupled with the Castep package to perform density functional theory (DFT) calculations, allowing us to calculate the formation energy of thousands of randomly generated structures. I began by performing calculations that randomly sampled the phase space in 5 GPa pressure increments from 0 to 25 GPa, and then plotted the formation enthalpies as a function of composition. I then calculated the formation enthalpy of Co_2C alone as a function of pressure and found that it was most stable around 7 GPa. After identifying that Co_2C could be stabilized by high pressures, we began preparing diamond anvil cells (DACs) for the synthesis experiments. In April 2021, we performed remote synthesis experiments at beamline 16-ID-B at the Advanced Photon Source, which allowed us to perform double-sided laser heating with in-situ XRD. The XRD data revealed new crystalline peaks above pressures of 4.8 GPa, which we identified to be Co_3C. This phase was not initially predicted by my computations. However, on account of the complexity of the randomly generated structures being limited by the number of atoms allowed per unit cell (9 atoms), the 16-atom Co_3C structure was not predicted. We published the results of this study in *Chemistry of Materials*.

Uncovering the Selective Reactivity of bis-N-oxide Caspase-6 Inhibitors Ethan Goulart '22



Currently, there are no cures for any neurodegenerative disease. Caspase-6, a cysteine aspartate protease, is present in the hallmarks of Alzheimer's Disease (AD) and Huntington's Disease (HD): amyloid-β plaques, neuropil threads, and neurofibrillary tangles. Caspase-6 is known to cause AD and HD by cleaving microtubule-associated proteins tau and tubulin, respectively. From a high-throughput screen, the Hardy Lab identified compound A (comp A), a bis-N-oxide, as a highly selective caspase-6 inhibitor. Comp A covalently modifies Cys-264, a non-conserved residue unique to caspase-6. Comp A, and its analogs exhibit a rare latent reactivity where they selectively modify one Cys in a sea of ten competing Cys in caspase-6. However, the mechanism of comp A reaction and the physicochemical basis for comp A's reactivity with specific cysteines remains unknown. In caspase-6, Cys-264 is adjacent to Lys-265, and we hypothesized that this Cys+ motif is necessary for comp A reactivity. To better develop bis-N-oxides as caspase-6 inhibitors, I investigated the physicochemical basis of comp A's selective reactivity in systems of increasing complexity from peptides to proteins. I synthesized six Cys+ containing oligopeptides in a background of varying hydrophobics and charges, incubated them with comp A and found no evidence of comp A modification via mass spectrometry. We concluded that comp A reactivity requires a more complex three-dimensional microenvironment likely provided in protein tertiary structure. To further uncover the extent of comp A's selectivity I incubated comp A with a series of Cys-containing proteins and determined the extent of binding or lack of binding via LC-MS. Additionally, using caspase-6 mutants, we uncovered key residues in the Cys-264 allosteric site that promote binding of our lead inhibitor via LC-MS and enzyme inhibition assays.

Synthesis of Traceable Cargo for Cell-Based Vehicle Systems Bao Le '23

Numerous platforms are being investigated for use as delivery vehicles, including nanoparticles, polymers, and conjugated antibodies. However, most of these accumulate passively, resulting in less than desired cargo accumulation at the target site. Cytokines generated in disease environments, including tumors, can serve as chemoattractants for multiple cell types, including macrophages and stem cells. The Farkas group proposes modification of cell surfaces for their use as imaging and active drug delivery vehicles, taking advantage of their disease targeting capacities. Towards this goal, fluorescent compounds are being synthesized as traceable entities with handles for cell conjugations, to evaluate linkages and effects on cells. My current study focuses on the synthesis of sulfonyl-N-hydroxysuccinimide (sulfo-NHS) and cyanine-5 (Cy5) to construct Cy5-sulfo-NHS for conjugation to macrophage surfaces. The attachment mechanism utilizes free lysines on cell surface proteins for conjugating moieties bearing NHS esters to the surface. The attachment of the Cy5-sulfo-NHS will be compared to the Cy5-NHS to analyze the effects of the sulfonyl group. By introducing a sulfonate on this leaving group, the entity being attached can benefit from improved solubility in media and avoid internalization due to the additional negative charge. In the future, fluorophores will be replaced with drug and/or chemical sensor cargo.

iCons by Wesley J. Dunham, iCons Strategic Communications and Program Manager

We are excited to announce that our name has changed to Integrated Concentration in STEM. iCons welcomes and includes students from across all disciplines in physical, life and natural sciences, engineering, public health, computer science, business, and technology. By replacing Science with STEM, we more clearly represent the diversity of students and faculty in the program while retaining the core focus on how students making advances in science, technology, engineering, and math contribute solutions to real-world problems.

Year 12 of the program brought a renewed sense of excitement and opportunity as we cautiously returned to campus. We welcomed the 12th cohort – the so-called "Carbon 12" cohort – in December, the largest and most diverse in the program's history, comprised of 73 students from 25 majors in five UMass schools & colleges, with 61% of students identifying as BIPOC.

The MicrobeBlaster team

Many iCons students received awards and accolades and we would like to highlight three graduating seniors for their efforts.

Sarah Kaunfer '22 (Microbiology) was honored as one of ten graduating undergraduates to receive a 21st Century Leader Award. Along with three fellow iCons students, she founded biotech startup MicrobeBlaster. Their team is developing an antifouling coating to prevent bacterial infection on implantable medical devices. Kaunfer also worked with Dr. Yasu Morita (Microbiology) to characterize the cell envelope of Mycobacterium tuberculosis, the causative agent for global respiratory disease. Upon graduation, Kaunfer will work as a clinical research coordinator in acute kidney injury at Brigham and Women's Hospital in Boston.

The iCons Program also boasts two UMass Rising Researcher Award recipients, **Benjamin Aaronson '22** (Biology and Spanish) in Fall 2021 and **Emily Leonard '22** (Biology and Public Health) in Spring 2022. Aaronson worked with Dr. Craig Albertson (Biology) researching the genetic basis of bone disorders such as syndactyly (fused fingers and toes) and how the environment affects bone development over time. Ben plans to study Spanish in Spain this summer to complete his dual degrees and will apply to medical school with the intent to work in sports medicine or orthopedics. Leonard worked in the lab of Dr. Alicia Timme-Laragy (Environmental Health Sciences) and researched the impacts of long-term dietary exposure to tBHQ, a synthetic food preservative, on zebrafish. Emily plans to attend Boston University School of Public Health to pursue a doctorate in Environmental Health.

We welcomed three new faculty members to our instructional team and said goodbye to **Dhandapani Venkataraman (DV)** of Chemistry, a longtime iCons 4 instructor who moved on from iCons to further his research on hybrid organic inorganic perovskites (HOIPs) and organic nanoparticles and their assemblies.

Joining us this year are **Wei Fan** (Chemical Engineering), **Erica Light '16**, **'22G**, and **Martin Hunter** (Biomedical Engineering). Light and Hunter co-instructed the newest iCons course, ICONS 390BH Integrated Discovery Lab in Biomedicine. This course, which is in collaboration with the Biomedical Engineering Department (BME) in the College of Engineering, serves as our iCons 3 course for the biomedicine/biosystem track. This pioneering laboratory course combines the key elements of iCons – interdisciplinary student teams, real-world problems, and student-designed innovation – with the world of biomedical science and engineering. Light is an iCons graduate, received her Master's degree in Sustainability Science, and is the 2021 recipient of the Mahoney Alumni Award. Light is interested in studying research ethics, the history of STEM fields, and how we can improve biostatistics. Hunter is a BME faculty member who brings experience with hands-on lab techniques that are typically not found in a standard life science laboratory, such as 3D printing, laser cutting, and casting and molding.

Wei Fan is the inaugural recipient of the iCons Teaching Fellowship, which brings talented and motivated instructors into iCons, and co-instructed ICONS 189H or iCons 1. Fan's research focuses on the rational synthesis of nanoporous materials, which serve as catalysts in biorefineries and drug delivery carriers.

The iCons Program has recently partnered with Impact Nano (located in Orange and Devens, MA) to provide development opportunities for promising undergraduates majoring in science, technology, engineering, and mathematics (STEM) through summer internships and part-time work throughout the year. Starting in May 2022, iCons students from several STEM majors will work closely with Impact Nano scientists, engineers, and operations personnel to scale up their new chemical manufacturing operation. The company makes advanced materials that enable breakthrough technologies in the automotive, semiconductor, and pharmaceutical industries. The company's location in Western Mass is strengthening the North American supply chains for these critical materials while also creating local jobs.

The Mahoney Alumni Award is given annually to an iCons graduate who exemplifies the mission of iCons. This year's recipient is **Jacob Lytle '16**. Lytle is a high school educator at Argosy Collegiate Charter School in Fall River, MA who uses the iCons educational approach and theory in his science teaching. Said one award reviewer, "Jacob uses ideas and principles that he learned in iCons in his own teaching. The fact that his students use their 'love of science to make the world better' is exactly what iCons is all about!"

We want to thank all our supporters and sponsors, including the Mahoney Family, the Chleck Family Foundation, Edward Marram '59 and Karen Carpenter, Impact Nano, Waters Corporation, VentureWell, Zipher Medical Affairs, iCAN (iCons Alumni Network), and all our benefactors.

We hope you will visit the iCons website, https://icons.cns.umass.edu, to keep up to date with our news and events and to check out student research projects on the Innovation Portal. We wish you all to stay safe, happy, and healthy.

Commencement 2022

Approximately 20,000 family members, friends and other guests cheered for a graduating class of about 7,000 under bright sunshine and warm temperatures at McGuirk Alumni Stadium on Friday, May 13th. Congressman Jim McGovern, who represents the 2nd District of Massachusetts, delivered the keynote commencement address, telling students: “I won’t tell you what to believe—but I will tell you that you have been given an incredible gift—a world class education. My question to you now is, what are you going to do with it?" Chancellor Kumble R. Subbaswamy recalled the many hurdles faced during the COVID-19 pandemic, commending the graduates: "Your perseverance and resourcefulness over the past two years is amazing."


Rep. Jim McGovern

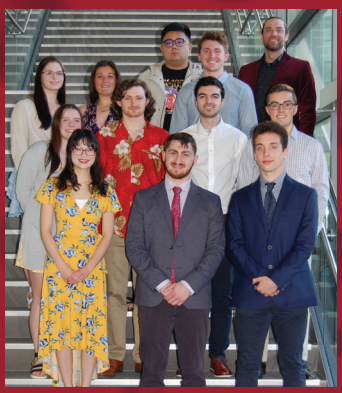

Chancellor Subbaswamy


Graduation Ceremony at McGuirk Alumni Stadium

The College of Natural Sciences Senior Celebration was held on Saturday at the Mullins Center, and the chemistry department hosted a Senior Recognition luncheon for graduates, family, and friends. Senior Ethan Goulart was nominated by his peers to be chemistry's CNS "chirper" and delivered a quick speech. Our Department Head, Prof. Ricardo Metz, Chief Undergraduate Advisor, Dr. Ruthanne Paradise, and Professor Michael Barnes led graduates to the stage, presented graduates with their CNS caps and commemorative medals, and congratulated them.

Chemistry 2022 Seniors: Laura Casey, Ziming Chen , Samantha Currie, Zachary Danaceau, Kevin Dillon, Adam Elmasri, Alexander Gauthier, Ethan Goulart, Deni Hamiti, Alexander Hill, Ellen Olivia Kernan , Owen Kuklinski, Joshua Lauterbach, Spencer Lawrence, Wenwei Liang, Guo Ling, Garrett Miskell, Hanna Ngo, Ryan Pham, Samuel Regan, Marissa Rizzi, Taral Shah, Sidrat Siddiqui, Mason Tomko, Mark Turner, Nhu Tong, Jikun Wang, and Jacque Moon Yee


Congratulations to all our 2022 Chemistry Seniors!!



Alumni Reflection: George Epstein '48

When I started at UMass in 1943 at age 16, I may have been the youngest in the freshman class. Today, as an alumnus (Class of 1948), I recently celebrated my 95th birthday. (I may be one of the oldest of the UMass alumni still around.)

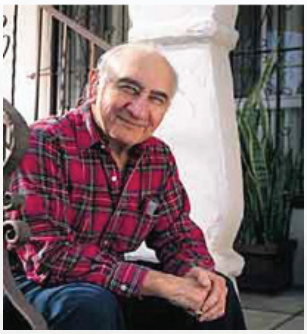


Photo credit: UMass Magazine

When I entered the freshman class in September 1943, little did I dream of how much my life would be affected. I owe my career, my wife and children to the school. Let me tell you how and why.

We were just recovering from the economic recession, during which my father had lost his shoe-manufacturing business and our house had been foreclosed on. Both my parents worked in a local laundry, and my father also managed the 6-unit building where we lived in Dorchester along with my younger sister. As a teenager, I often helped my father on his laundry truck. In fact, that was when he taught me to drive his truck.

When I began my college education, I had no real idea of what sort of career I would pursue. Perhaps a medical doctor. That would please my parents. So I registered for freshman chemistry along with four or five other classes. My freshman chemistry teacher was Dr. J. Harold Smith, a recent PhD graduate of the University of Wisconsin. That experience pointed me in my career direction.

Our textbook, *Principles of Chemistry and Reference Book of Inorganic Chemistry* by Joel H. Hildebrand (5th printing, 1941) was so heavy, it was a burden to carry to class. Professor Smith made the class so exciting and interesting that I soon found myself spending much of my spare time in the Goessmann chem lab, designing my own experiments. That led to an interesting experience. After one of our frequent exams, my paper was returned to me showing one question marked wrong. But that question was about an experiment I had run during one of my frequent visits to the lab. After class, somewhat nervously, I went to his desk and told him so. "Let's march right over to the lab and see," he responded. As the professor watched, I mixed the ingredients. Sure enough, there was an immediate reaction as a precipitate formed in the test tube. Professor Smith gave me a big smile as he explained, "perhaps it has to do with the concentrations." Then, he added, "I will change your exam grade to 100%."

The next semester, I became a Laboratory Assistant in the Analytical Chemistry Lab where I would work to prepare unknown solutions for analysis and help the other students to solve their assigned problems. The pay supplemented my full-tuition scholarship.

I also became a reporter for the Sports section of the campus newspaper, *The Collegian*. Later, I was promoted to Sports Editor. In that capacity, I had the opportunity to work with the student group advocating for raising Mass. State College to the university (UMass). We all celebrated when the change was announced in 1947.

While living in the boy's dormitory in North Hall (and later in the fraternity house), I enjoyed playing poker for pennies with other students. That recreation – providing mental challenge and social interactions – continued in later years; and, when I retired from my career as a materials specialist contributing to the fast-growing aerospace industry, I decided to make poker my "second career."

I joined one of the school's fraternities, Tau Epsilon Pi (TEP), and made many new friends. I thoroughly enjoyed the social interactions. To help pay my dues, I worked at the fraternity house, helping to serve the food and cleaning up. One of my roommates, Joe Cohen (later changed to Casden), who was struggling with the technology classes, hired me to tutor him. In return, Joe gave me sandwiches from his family's food market. Joe and I remained good friends for many years; he became a successful CPA.

Another dear friend from the fraternity was Art Karas who later got me involved in a profitable bus service business to transport students from Boston to the school and back again.

I played on the school's baseball team in several positions. Catcher was best because I was involved with every play. I also enjoyed playing first and third bases. We played against teams from other local colleges. The summer of my sophomore year, a group of college professors challenged us in a baseball game. It is still vivid for me how I slid into second base while it was guarded by Professor Walter Ritchie, Chairman of the Chemistry Department. I ran from first base as fast as I could and slid as hard as I could, knocking Professor Ritchie to the ground. *Oh my,* I thought, *what have I done?* I leaped to my feet to help him up. He smiled and told me he was alright. Phew!

After the first semester of my junior year, I was inducted into the US Navy. World War II was underway. Because of the technical skills gained at MSC/UMass, I was trained as an electronics specialist and put in charge of maintaining the radar, loran, and sonar on a destroyer/minesweeper patrolling the Atlantic Ocean. Mostly we escorted or towed other ships that were experiencing engine anomalies, helping them to get back into port for repairs. Most exciting and rewarding was how I was able to repair our ship's radar that had previously often failed while at sea, necessitating that our ship return to port for repair by the manufacturer of the equipment. Shortly after I came on board, our ship's radar failed again. So I put some of my college training to work by analyzing the likely causes and carefully inspecting the parts involved. I observed a large vacuum tube – the cathode – essential to the power supply, with a phenolic plastic insulation section broken away. Removing the tube for closer examination, I noted that the metal behind the insulator was darkened – presumably oxidized while operating in the high-humidity ocean environment. So I sanded the corrosion way and reassembled the tube. Lo and behold, when I turned the radar back on, it worked perfectly. I had solved the nasty problem that had troubled our ship for so long! After that experience, I soon found myself loaned out to other Navy ships experiencing electronic malfunctions.

I was put in charge of replacing our ancient loran set using more modern equipment. One day, as we headed to port, our radar started squeaking. The Captain summoned me. "We cannot go into port until we stop the squeak," he ordered. Gathering lubricating equipment and several rags, I climbed

the mast with my two assistants following from behind. At one point, a piece of rag got loose and started a long drift down into the ocean. I watched. *Scary*, I thought, and held on tighter to avoid falling. All it took was a few squirts of lubricant on the right spots, and there were no more squeaks.

Soon the war was over and I was able to return to UMass under the GI Bill to complete my studies. In October 1947, I was voted into the honor society, Phi Kappa Phi. Then, in June 1948, I was conferred with my BS degree Magna Cum Laude, ranking first in the Chemistry class.

For my graduate work in chemistry, MIT offered me a partial scholarship which, along with the remainder of my GI Bill, would cover my first year's tuition. For my other expenses, I worked part-time as a Research Fellow in the Plastics and Adhesives Lab on an Army contract to study the thermal degradation of adhesive bonds.

These and other good things happened to me from then on; and I believe it was because of the learnings and experiences during my years at MSC/UMass. Let me summarize:

For the summer months before starting at MIT, I enjoyed my vacation at our family summer home in Nantasket Beach and developed a laundry pick-up and delivery route. Each evening, my father would take whatever laundry I had picked up from my customers, bring them to the laundry where he worked, and when ready, return to me for delivery to my customers – and keep the profits. I had fliers printed up and, with the help of a few local teenagers, distributed the fliers to potential customers in the area. Before long, I had a significant number of viable customers, including two local hotels, and many summer vacation houses. I spent the mornings on my new laundry services business, and the afternoons were great for enjoying the beach just a few blocks from our family summer home.

And that's how I met Irene. Her family had a summer vacation home in Nantasket Beach. One of my best customers, Mrs. Buxbaum, asked if I could drop her off where she could settle a bill. As we drove there, she pointed out the house. As we chatted in the doorway with Mrs. Tabrisky, a door opened from the second floor – and out walked a "vision of loveliness" as I watched her climb down the stairs. Soon after, our romance began; we later married in Los Angeles. It was on July 4th – a national day of celebration.

While at MIT as a graduate student/research fellow, I studied the effects of elevated temperature on structural adhesives. Then, in cooperation with Professor A. G. H. Dietz, I wrote my first published technical paper for the ASTM Journal. (This may well have been a factor in my selection as a Research Engineer at North American Aviation after completing my studies at MIT.)

After graduating with my MS from MIT, I went to work in the fast-growing aerospace and defense industry, where I was able to contribute to key technologies as part of a number of major programs. These included missiles such as the Polaris and Titan launch vehicles, space communications satellites such as NATO III and FleetSatCom, and the Global Positioning Satellite (GPS)

At North American Aviation, I was responsible for developing the first high temperature structural adhesives. This technology is used today in film adhesives in aircraft and space systems. My book, *Adhesive Bonding of Metals*, published in 1954, was the first on structural adhesives, and was copied into Russian.

As assistant chief engineer of the Structural Materials Division at Aerojet-General Corp., I contributed to the development of high-temperature thermal insulations for rocket motors and impermeable liners for pressure vessels, materials for filament winding, and metal/fiberglass laminated structures. My team developed the tensile test method for fiberglass rovings, and the concept of laminating thin metal sheet with alternating plies of unidirectional fiberglass, the precursor to the GLARE material used in the Airbus A380 aircraft.

Working for The Aerospace Corporation from 1966-1991, I introduced advanced composites into US Air Force space systems. At the time, the Air Force discouraged the use of advanced composites in favor of metallic structures. Because weight is a major limiting factor in the design of space systems, I gained support from the Air Force Materials Laboratory for an extensive R&D program to develop design data and demonstrate feasibility. Subsequently, I led a team of engineers in monitoring/supporting the development of the narrow beam precision horn antennas and mounting structure for the NATO III communications satellite consisting of thin carbon/epoxy facings bonded to low density honeycomb core. The success of this effort led to the extensive use of advanced composites in other Air Force and NASA space programs.

Having been involved in resolving many problems for Air Force Space Systems, as the Director of the Manufacturing Engineering Office at The Aerospace Corporation, I established the Air Force Manufacturing Problem Prevention Program (MP3) with team members from Air Force contractors to disseminate lessons learned in order to prevent recurrence. I also contributed to the Air Force Space and Missile Systems Center Commander's policies to prevent such problems.

During that time, I participated in several engineering societies, holding high office and contributing to their programs to enhance and apply special materials technologies. In fact, The Society of Plastics Engineers, So. Cal. Section, has a scholarship in my name, and The Society of Advanced Composites (SAMPE) in cooperation with The Air Force Space Systems Division, honors my late wife by awarding college scholarships to high-school seniors, which is now in its 26th year.

As mentioned, upon retirement from The Aerospace Corp., I decided to make the game of poker my second career. It had been my hobby for recreational diversion while at MSC/UMass. To date, I have authored three poker books, written hundreds of poker columns for a number of publications, organized a seniors poker group, and presented extensive courses and lectures on playing winning poker for a wide variety of organizations. My focus is on poker as recreation for retirees, providing them mental stimulation and social interaction.

During the coronavirus pandemic, I have been playing poker online and have earned well over one million in points – not money.

My days at UMass taught me the knowledge and gave me the experience that led to all these wonderful things happening to me along the way.

Alumni

SUNY Lecture Hall Named After Silveira

Dr. Augustine Silveira (PhD '62, with Earl McWhorter), BS '57, ScD (Hon) '75 UMass Dartmouth taught chemistry at SUNY Oswego for 38 years, and was department head for 34 of those years. He retired over twenty years ago, but he and his wife, Beverly, have continued to make contributions in education. In appreciation of their devotion and donations, SUNY Oswego named the Dr. Augustine and Beverly Silveira Lecture Hall in their honor.

"Having grown up in the Depression, I knew my family could not afford to send me to college. I held four jobs throughout my undergraduate years. I vowed that when it became possible, I would do everything I could so that the best students would not have to work as hard as I did while earning a degree," Dr. Silveira said.

We congratulate Dr. Augustine and Beverly Silveira, and thank them for their generous educational support, including gifts to UMass Chemistry.

Checking In with PhD Alumni: Faculty Focus

Every year, 20 to 30 new students from all over the world join our Chemistry PhD program to continue their education, pursue their passion for chemistry, and prepare themselves for a career in science. After they have finished their coursework, made it through their prospectus and ORP exams, discovered some fascinating new chemistry, passed their data defense, and successfully celebrated their final defense, they are ready for a new career in the "real" world. Most PhD chemists from our Department eventually take positions in companies, but some students seek a job at a university or college to train the next generation of scientists.

The following chemistry PhD grads started faculty positions within the last five years. We asked them why they chose a career in academia, and how UMass prepared them for their current positions. Here's what they had to say.

Nicholas Borotto, PhD 2016 (Vachet group), Assistant Professor, Department of Chemistry, University of Nevada

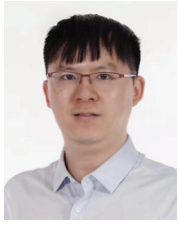
I was drawn to academia for two major reasons: 1) the freedom to pursue and publish on the topics I find most interesting; and 2) to mentor the next generation of early career scientists. The University of Massachusetts provided an excellent environment to grow as an early career scientist. It fostered the development of numerous skills required of academia (e.g writing and mentoring). The excellent community of graduate students advanced my networking and softball skills. But most importantly, my time at UMass began to give me the confidence and resilience that is necessary to prosper in the academic environment.

S. Gokhan Elci, PhD 2016 (Vachet group), Assistant Professor (2018-present), Department of Biomedical Engineering, Pamukkale University, Turkey

It seemed like a long journey from the beginning to the end of my PhD with many challenges and happy memories along the way, but eventually, I got what I have always dreamt of, and I have started as an assistant professor in Biomedical Engineering Department at Pamukkale University, Turkey. Since high school, my dream was always to become an academic. My father, a retired chemistry professor, was my inspiration, and he is a great example to me on this journey. Like my father, my sister is also a chemist and academic, which made me think of continuing the family tradition as well. I have always liked science since high school, and it is the driving force for me to seek new things and learn what is new in science. The best career to keep up with that knowledge is to become an academic. So far, with two great and insightful academic fathers (both my dad and Prof. Richard W. Vachet), I know that I made the best choice to be a professor. The idea of passing knowledge to younger science enthusiasts is fulfilling and it's a great feeling to be in this job.

Ying Jiang, PhD 2016 (Rotello group), Assistant Professor, College of Chemistry, Beijing Normal University

I enjoy the freedom of researching problems that captivate me and working with young and well-educated students that bring fresh ideas. I also enjoy the mentorship aspect of teaching. So, being a professor is the best outcome I have hoped for. Studying at UMass has shaped me to be self-confident, independent, and persistent in a way that I will forever be grateful for. I believe the cultivation of these essential traits helped prepare me for being a professor.



Longyu Li, PhD 2015 (Thayumanavan group), Professor, College of Polymer Science and Engineering, Sichuan University

My time at UMass was a great experience. I met many great professors, including my advisor Thai, and my committee, Kevin and Min. I also remember that I took many useful classes from Richard, Scott, Vincent, Nathan, DV, and others in the first year. I came to the US for my PhD with the goal to be a professor. At that time, I thought being a professor was a great job, as one can arrange their schedule independently. Now, I believe that it is a pleasure to work with young students and postdocs, developing interesting projects from a seed to a tree. My experience at UMass helped me realize this point. I saw many

professors who genuinely cared about their students. I could not achieve my current position without help from Thai.

Patanachai 'Kong' Limpikirati, PhD 2020 (Vachet group), Lecturer, Department of Food and Pharmaceutical Chemistry, Chulalongkorn University, Thailand

Before going to UMass, I wanted to work in academia because of my love for teaching and my childhood dream that I wanted to be a teacher. UMass Chemistry helped strengthen my basic knowledge, trained me how to conduct research, and shaped my soft skills and respect for diversity and equity. Over years at UMass, I realized that being a professor is a purpose of my life to improve the field of Pharmaceutical Analysis through research and outreach and to serve my students. I always remember my professor saying that "A big part of being a good teacher is caring for your students and being willing to help them in the way that works best for them."

Alyssa Marsico, PhD 2016 (Vachet group), Assistant Professor, Dept. of Forensic Science, University of New Haven

I became a professor because I love sharing my passion of science to both developing scientists and experienced scholars, and because I always enjoy coming up with innovative ways to explain complicated scientific material. I had the opportunity to do these at the University of Massachusetts at Amherst. One of the largest influences on my decision to become a professor was the welcoming environment at UMass Amherst that fostered scientific discussions between graduate students in other disciplines of chemistry, and even the faculty who were always open for a conversation. Other influences were the experiences I had both mentoring new research students, and all the opportunities provided to present my own research. Both allowed me to share the knowledge I was gaining while at UMass Amherst. These experiences made me realize that I enjoyed just talking about chemistry in general and sharing my own expertise and passion in the field to both new and established scientists, which I continue to do now as a professor.

Bach Pham, PhD 2020 (Min Chen group), Assistant Professor, Department of Chemistry, University of Science, Vietnam National University

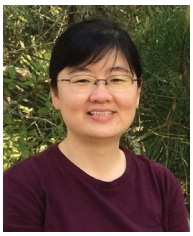
Since the pandemic, life science has grabbed much attention, yet it is still an undeveloped research field in Vietnam. Meanwhile, chemistry students at my university focus on classical chemistry and do not have access to biochemistry knowledge, which limits them from studying life science. Thus, I would like to contribute what I have learned about biochemistry and life science at UMass, equip students with fundamental knowledge, and introduce them to advanced research directions in this field.

Satamita Samanta, PhD 2013 (Martin group), Lecturer (2021-present), Dept. of Chemistry, University at Buffalo

I find teaching incredibly rewarding. I get to talk to students about my favorite subject, connect the pages on their books to everyday life, introduce young minds to research, and see their interest in chemistry grow. UMass gave me the first opportunity to experience teaching and made me realize my love for teaching and mentoring!

Cornelius Taabazuing, PhD 2015 (Knapp group), Assistant Professor, Department of Biochemistry and Biophysics, University of Pennsylvania Perelman School of Medicine

I'm currently an Assistant Professor in the Department of Biochemistry and Biophysics at the University of Pennsylvania Perelman School of Medicine. I decided to become a professor because I love discovering new things that have the potential to impact humanity in a positive manner. My undergraduate and graduate education at UMass Amherst had a major impact on my career decision. I was instilled with a curiosity about how the natural world works that still drives me today. I had the opportunity to participate in research during my junior year as an undergrad and absolutely fell in love with it! The combination of fantastic mentors and phenomenal educators, exposure to diverse research areas, and excellent curriculum at UMass prepared me well for life as a faculty member.



Yi-Cheun Yeh, PhD 2014 (Rotello group), Assistant Professor, Institute of Polymer Science and Engineering, National Taiwan University

I became a professor because I enjoy active discussions with people about science, especially brainstorming for problem-solving and making new molecules/materials. Doing research is a lifestyle for me, and I love it! The pleasant working environment and the diverse international student community at UMass helped me to pursue my passion for science and to achieve the goal of becoming a professor.

Please keep in touch!
Update your mentor and consider submitting an article for the alumni section. We'd love to hear from you!
ggazette@umass.edu

Industry Focus in the next issue will center around PhDs and undergraduates who chose industry positions.

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"Being named the recipient of the Thomas R. "Casey" Stengle scholarship allowed for me to further fund my education and focus primarily on my passion for chemistry and computational chemistry research within the Auerbach lab."

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Cheng-Yi Wu '72 PhD & Jane (Wang) Wu '72 MS
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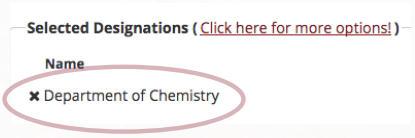

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Pushing the Frontier of Quantum Chemistry

Ethan French '23 was recognized as a 2021 UMass Rising Researcher for performing outstanding research and exercising exceptional creativity. He transferred to UMass Amherst in his sophomore year when all his classes were online and found a remote research position in a computational chemistry lab, a new area for him. At first he felt as if he was "being thrown into the deep end" and was unsure if he had made the right decision. He soon discovered he had. In the lab of Assistant Professor of Chemistry Zhou Lin, which focuses on the development and application of fragment-based quantum chemistry techniques, French says he "fell more in love with chemistry as I was exposed to a part of it that I didn't know existed."

Lin praises French's impressive progress. "He has a unique dual background in chemistry and programming, allowing him to appreciate problems in chemistry and to program theory into codes," she says. "His projects push the frontier of quantum chemistry by accelerating existing approaches without compromising accuracy."His current research involves the application of machine learning to chemistry. Most recently, he used machine learning to predict quantum mechanical properties of molecules. These calculations are extremely important for computational materials and drug screening, among other things, he explains. However, they are costly and time consuming; some calculations require multiple days. French helped successfully reduce the process from approximately 12 hours to about 90 seconds.

As a result of his work in Lin's lab, French was the second author on a paper published in *The Journal of Physical Chemistry Letters*. Lin expects that his ongoing work will result in at least two more publications. French also received the Department of Chemistry's 2021 Uche Anyanwu Memorial Award at the annual Undergraduate Research Poster Session.

As a hard-working and highly motivated student, French values his mentor's advocacy. For example, he says, "Professor Lin often sends emails to alert us to opportunities and encourage us to pursue them." He believes his work in Lin's lab has kept him "constantly curious."

"There is always more to know," he says. "Research has also given me a chance to focus on an area of chemistry that I can now see as being a part of my career."