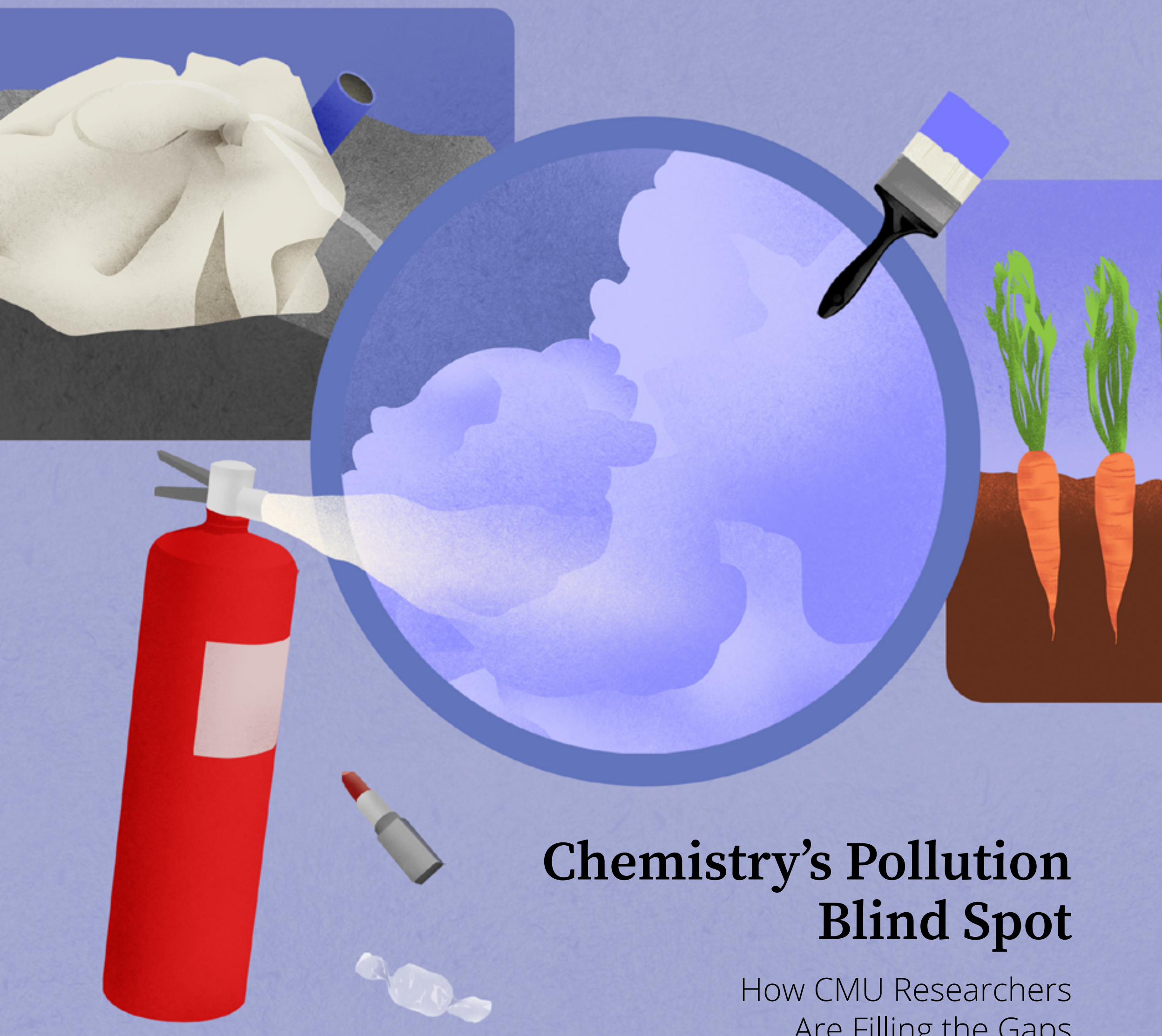
2025

THE INITIATOR



Chemistry's Pollution Blind Spot

How CMU Researchers Are Filling the Gaps

Carnegie Mellon University
Mellon College of Science
Chemistry

THE INITIATOR

The Department of Chemistry

The Initiator is published yearly by the Department of Chemistry at Carnegie Mellon University for its students, alumni and friends to inform them about the department and serve as a channel of communication for our community. Readers with comments or questions are urged to send them to army@andrew.cmu.edu. The department is headed by Bruce Armitage.

Editor-in-Chief
Bruce Armitage, Department Head

Editor
Heidi Opdyke, Associate Dean for
Marketing & Communication

Design & Layout
Samantha Zemanek, Graphic Designer

Contributing Writers
Bruce Armitage, Stacey Federoff, Kirsten Heuring, Amy Pavlak Laird, Heidi Opdyke, Ann Lyon Ritchie, Lauren Smith, Elizabeth Speed, Yi Tang

Photography & Images
Jonah Bayer, Digital Producer
Courtesy of Carnegie Mellon University, unless otherwise noted

Online Magazine
Gigi Wiltanger, Web Manager
Iulia Dumitriu, Web Content Administrator

The Department of Chemistry
Carnegie Mellon University
5000 Forbes Avenue
Pittsburgh, PA 15213
www.cmu.edu/chemistry

Scan code to view online version of The Initiator.

Contents

Dear Alumni, Friends and Family,

As we bring another academic year to a close, we're happy to bring you another edition of The Initiator, where you'll find the latest news from the Department of Chemistry. In addition to exciting new advances, the Research Feature on sustainable chemicals highlights our department's growing commitment to a safer approach to chemical design and synthesis. We've also instituted a staff profile in this year's magazine, with the spotlight on Lorna Williams-Rolley, the glue that holds our graduate program together. It has also been a great year for our graduate students, with new NIH, NSF and Rales Graduate Fellows in (or soon to join) the department in addition to several CMU and MCS fellowship and award winners.

As successful as this year has been for us, it is also a time of great concern. I recently attended a meeting of chemistry department heads from 26 universities. Common themes were budget deficits, canceled research grants and scaled back admissions to graduate programs due to a changing federal funding landscape that threatens to reduce support for university-based research by up to 50% in the coming year. Federal funding serves two main purposes. First, it advances the frontiers of knowledge by supporting the kind of open-ended, fundamental scientific investigation that industrial labs rarely pursue. Second, it supports the training of the next generation of scientists who will not only become future faculty but also drive innovation in the chemical, biotechnological and pharmaceutical industries. These cuts will severely harm our nation in both the short- and long-term.

You can make an impact in two ways. First, write or call your elected representatives asking them to stand up for science by opposing cuts to agencies like the National Science Foundation and National Institutes of Health that support the majority of research at universities like CMU. Second, consider making an unrestricted donation to our department. Alumni donations provide an essential resource that the department can tap into in cases like this. In fact, gifts to our department nearly doubled in the last two years. As reluctant as I am to ask for more, the red lights are flashing. I hope what you read in this edition of The Initiator convinces you that any contributions will be used well by the amazing faculty, staff and students in our department.

Finally, as bittersweet as it is to say goodbye to the most recent group of graduates, we also bid farewell to Professor Karen Stump, who guided our undergraduate program for the better part of four decades and now transitions to her retirement. Karen's teaching and mentorship extended far beyond students in the classroom and lab to our instructional staff and faculty. Karen's office (with those ever-filled candy jars) was a frequent destination for me as I tried to find my own voice as a teacher. She will be deeply missed.

Thank you for reading, and thank you for giving.

Bruce Armitage
Head of the Department of Chemistry

Department Notes

CMU-Q Faculty Member Awarded GAITAR Fellowship

Nimer Murshid is researching how generative AI tools can be used to improve teaching and learning in undergraduate coursework.

Murshid, an assistant professor in the Department of Chemistry based at Carnegie Mellon University in Qatar, received a fellowship from Carnegie Mellon's Eberly Center for Teaching Excellence and Educational Innovation in fall of 2024.

The fellowship is part of CMU's Generative Artificial Intelligence Teaching as Research (GAITAR) Initiative, which measures the impacts of AI tools on student learning and educational experiences.

Murshid, who joined Carnegie Mellon in the fall 2023, is investigating if AI tools can enrich learning in non-major elective courses like chemistry.

"At the heart of this initiative is the observation that learning is a unique journey for each student," Murshid said. "Through this investigation, I hope to see if AI tools can personalize education more effectively, catering to individual learning paces and needs."

Murshid is exploring whether these AI tools have different impacts on students from different academic disciplines when learning the same topic.

The GAITAR Fellowship provides $5,000 for a Carnegie Mellon instructor to design and implement a teaching innovation using a generative AI tool in a course. They must then measure the impacts of the innovation on student learning and disseminate their findings at the university and beyond.

Carnegie Mellon has a rich history for blending science, AI and machine learning, and CMU remains at the forefront of AI research. The work to apply generative AI tools and techniques in the classroom is one part of a broader university strategy to advance the next generation of artificial intelligence's impact across education, research and society.

■ *Angela Ford*

Unbreakable Bonds

Generations of Students Learn from Stump's Guidance

The room was packed with students attending a wellness workshop on ways to deal with stress. Angie Lusk from Carnegie Mellon University's Division of Student Affairs led the discussion.

"What do you do in times of real challenge?" she asked.

A voice called out: "You go to Karen Stump's office!"

It's good advice — just ask any of the many, many students who know the highly regarded teacher, mentor and advisor.

For the past four decades Stump, a teaching professor and director of undergraduate programs in the Department of Chemistry, has advised hundreds of chemistry majors and taught thousands of students, including chemistry, biology, engineering and pre-health students. As she heads into retirement, there's no doubt that she has made a lasting impact.

"I would want everyone to have an advisor experience like I had with Karen," said Chemistry alumna Erin Gantz, who graduated in 2010. "There is just something about her. She cares deeply about how you're doing as a person. You would go and meet with her, and it would seem like she had all the time in the world for you."

Stump, who graduated from Carnegie Mellon in 1981, returned to the Department of Chemistry in 1983 as a laboratory instructor after spending a few years teaching at Washington and Jefferson College. At the time, there were no women in the department, and a faculty teaching-track wasn't yet an option. But Stump loved teaching, meeting and talking with students, so she forged her own path.

"Looking back, I was creating a career, but I didn't realize at the time that was what I was doing," Stump said. "I would look at things that needed to be done, and I would just kind of start doing them. You're only limited by your own creativity and energy."

Stump has had plenty of both. In addition to teaching and advising, she started a teaching assistant training program, and she brought order to the undergraduate labs by organizing equipment, keeping a detailed inventory and leading staff meetings. This led to the creation of a new position — director of laboratories — for Stump. When it became clear that the labs needing renovating in the late 1990s, Stump rolled up her sleeves and got to work, collaborating closely with the architects designing the new space. The project was completed in 2003.

"It was quite an undertaking, to even think about building a lab that you know will not be rebuilt for literally decades and to think about what students will need in order to be successful for things you can't even imagine."

She also was responsible for administrative oversight of the undergraduate program in chemistry, led educational outreach activities and has been deeply involved in curriculum development for chemistry and the Mellon College of Science.

For her efforts, Stump has won three university-level awards: the 2017 Teaching Innovation Award, the 2011 Award for Outstanding Contributions to Academic Advising and Mentoring and the 2005 William H. and Frances S. Ryan Award for Meritorious Teaching. She also is the 2024 recipient of the Richard Moore Education Award in the Mellon College of Science.

The mother of three and grandmother of two has juggled a lot over the years, and it's that experience — along with a detailed knowledge of the ins and out of what's required to earn a chemistry degree — that has made her so valuable as an advisor.

"I've had students who come to see me pretty regularly for what they call their life-crisis talks. Sometimes it's personal, and sometimes it's academic. I've had students say: this is going to be a long one because I just need to talk out some stuff, and you're the person I do that with, so I need you to solve my life today."

Her overarching advice? Life is a journey, not a destination. Stump said she has lived that philosophy, and she spends a lot of time trying to convince students to live their lives a bit more that way.

Stump has been easing into retirement as she shepherds one last group of advisees through to graduation. She's looking forward to spending more time with her family, including going to the movies with her husband and taking the dogs to pick up the grandkids at the bus stop. But it's a bittersweet time for Stump, as she also has her extended family — her students — to think about.

"I think I get through it simply because — and I always say this at graduation — that I expect that we'll keep in touch. You'll let me know when you can how you're doing. And a lot of them do," Stump said. "I'm just so amazed at the types of things they're doing. I'm really proud of them."

■ *Amy Pavlak Laird*

Students pose alongside Karen Stump at the celebration of her last day at CMU.

Kurnikova Wins Distinguished University of Pittsburgh Alumni Award

For CMU Chemistry Professor Maria Kurnikova, things have come full circle. As a graduate student at the University of Pittsburgh, she spent so much time in a basement lab working on a state-of-the-art SGI workstation that her advisor, Professor Rob Coalson, often wondered whether she still existed. These days, Kurnikova said she rarely sees graduate students in person because everyone floats in cyberspace.

Kurnikova, who earned her doctorate from Pitt in 1998, received a 2024 Department of Chemistry Distinguished Alumni Award from Pitt. She accepted the award at a ceremony in September 2024 in recognition of her accomplishments and contributions.

Kurnikova's group specializes in developing theoretical computational models to determine the structure-function relationships in biological macromolecules. Her approach uses a combination of physics-based computational methodologies, such as molecular dynamics simulations, continuum electrostatics and quantum chemistry, as well as machine learning methods. Running these simulations requires high-performance computing tools, so she uses national supercomputer facilities like the Pittsburgh Supercomputing Center.

She is particularly interested in studying how the structures of membrane-associated proteins and protein complexes dictate their function in signaling and ion transport. These proteins remain relatively poorly understood despite being crucial for medicine, pharmaceutical science, environmental sciences and bioengineering.

Since joining the Carnegie Mellon faculty in 2003, Kurnikova has developed models to understand a variety of membrane-associated proteins, including glutamate receptors and NMDA receptors as well as the bacterial toxin alpha-hemolysin and the diphtheria toxin. Co-director of the Molecular Biophysics & Structural Biology Graduate Program at the University of Pittsburgh and Carnegie Mellon, she also is developing high-throughput approaches for structure-based in silico drug design.

■ *Amy Pavlak Laird*

TAML Catalysts Efficiently Break Down Pharmaceuticals in Polluted Waters

CMU scientists have found that an environmentally friendly process involving a TAML catalyst and hydrogen peroxide effectively degrades several antibiotics and other drugs found in municipal secondary wastewater and contaminated river and lake water. The drugs are representative of the hundreds of chemical micropollutants of concern found globally in wastewater as well as in rivers and streams that supply drinking water.

“This work presents a low-cost, broadly applicable, safe and sustainable solution for purification of pharmaceutical-contaminated waters using an extremely low concentration of catalyst and peroxide,” said Terry Collins, the Teresa Heinz Professor of Green Chemistry and Director of the Institute for Green Science at Carnegie Mellon.

The results, published in the journal ACS Sustainable Chemistry and Engineering, show that a next-generation TAML catalyst, called NewTAML, exhibits unprecedented efficacy in activating hydrogen peroxide (H_2O_2) at ultra-low concentrations. Because of a quirk with the catalyst — it lasts longer and does more work as its concentration is lowered — the amounts of TAML and H_2O_2 needed to run the entire process can be dropped substantially in consequence, which ultimately will reduce operating costs.

Past studies with TAMLs have shown their enormous potential to provide clean, safe, more effective alternatives to existing industrial and commercial practices and to provide ways to remediate other pressing environmental problems that currently lack solutions.

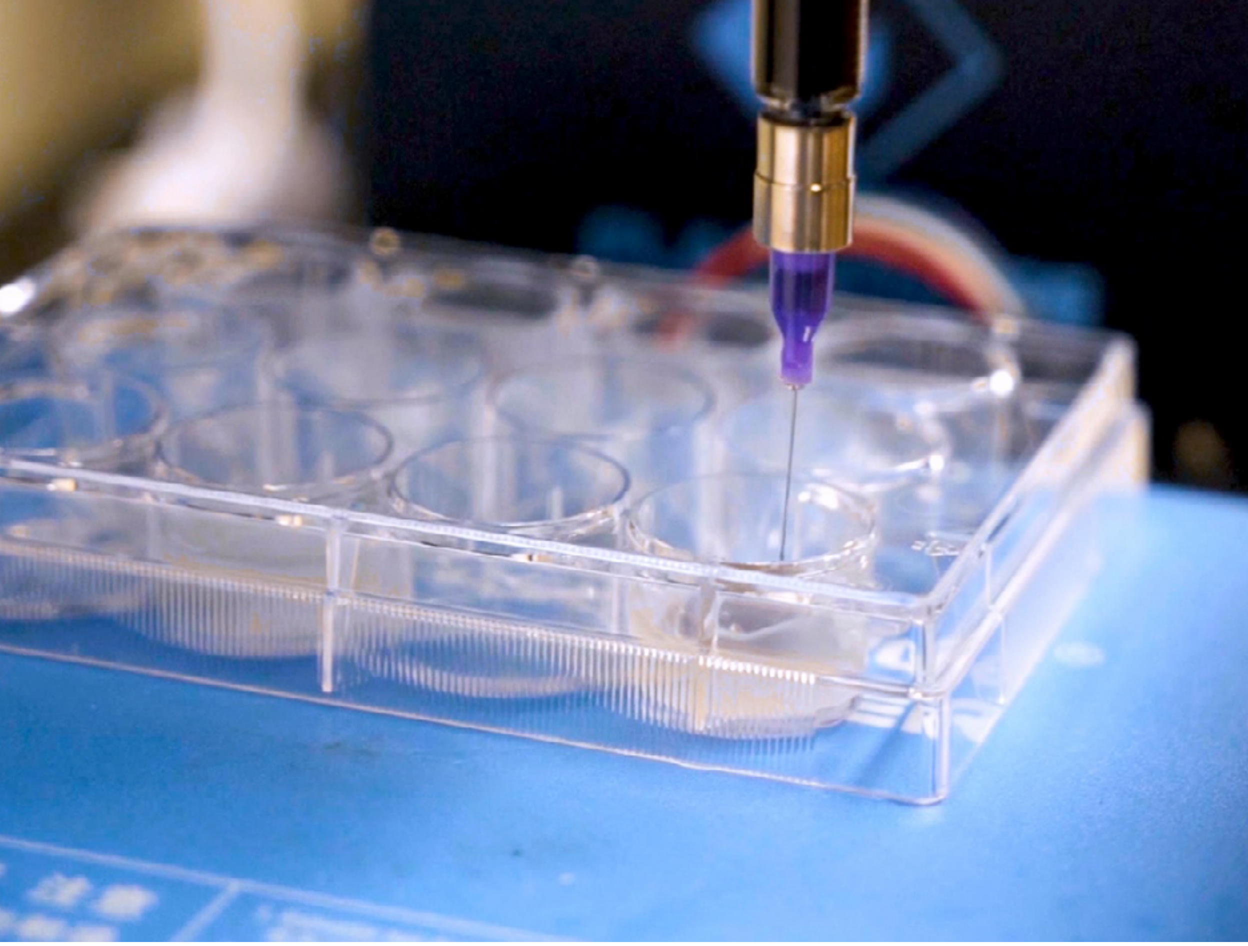
■ *Amy Pavlak Laird*

ISAYEV NAMED INAUGURAL CARL & AMY JONES PROFESSOR OF INTERDISCIPLINARY SCIENCE

CMU Professor Olexandr (Oles) Isayev uses interdisciplinary approaches to drive rapid advancement in the field of drug discovery and materials science. He has been named the inaugural Carl & Amy Jones Professor of Interdisciplinary Science.

Isayev joined the Department of Chemistry as an assistant professor in 2020. He is joint appointed in the Department of Materials Science and Engineering and affiliated with the Department of Computational Biology.

The chair is named for 1956 Mellon College of Science alumnus Carl Jones and his wife, Amy. Through a generous gift they established an endowment that supports the chair and the Future of Science Initiative through interdisciplinary collaborations and the Carl & Amy Jones Lecture in Interdisciplinary Science.



CMU Startup Helps Formulators with Complex Design Problems

Ansatz AI developed a digital chemistry tool to help companies design products to be less expensive, more sustainable and perform better.

Working with development partner Procter & Gamble, Carnegie Mellon University startup Ansatz AI recently announced the release of Hierarchical Machine Learning (HML) software. Designed for personal care and consumer products, this powerful tool makes design and optimization of a diversity of formulated products simple.

The startup was founded by Newell Washburn, an associate professor of chemistry and biomedical engineering with a courtesy appointment in the Department of Materials Science and Engineering; and Barnabas Poczos, an associate professor of machine learning.

"I was always interested in designing molecules and materials to have a certain function and wondered if we could use machine learning to do so if we didn't have a lot of data," Washburn said.

Washburn and Poczos discussed how to use machine learning to analyze sample sizes as small as 20 to 30 items rather than sample sizes of hundreds or thousands. Along with the help of students, they built HML, a data processing system for analyzing data records in designing a formulation of a material. The system's development was supported by an NSF grant.

Through resources in Carnegie Mellon's entrepreneurial ecosystem, the researchers patented their work and licensed it through the Center for Technology Transfer and Enterprise Center (CTTEC). The center guides faculty and students through the process of transferring invention to industry where they can be developed into commercial products. Washburn also consulted with contacts in Carnegie Mellon's Project Olympus, which offers faculty and students startup advice, microgrants, incubator space and connections to turn research and ideas into businesses.

Ansatz AI began as a consulting firm and has worked with companies in the United States, Europe and Japan on a diversity of problems in molecular design, formulation and process optimization. Calvin Gang, Ph.D. student, Ansatz co-founder and chief system designer, took that process and built an interactive design tool.

"The critical piece for us is that we ask our clients a lot of questions about how something works and what chemical interactions control results, and how you model that," Washburn said.

Ansatz AI's platform helps clients by providing a systematic framework for understanding how various compounds may work together based on their properties. Once the platform has been provided candidate chemical forces and interactions, it builds a model for how the product works. Based on that model, formulators can virtually experiment by adjusting the amounts and types of compounds before identifying a limited number of formulations to test in real life.

Behind the name

Ansatz in German means "best guess," and in English the word is used in math and physics to describe the starting point to solve a problem.

Carnegie Mellon University and its startup companies are committed to engaging with US industry in solving a broad range of technological challenges.

■ *Heidi Opdyke*

DID YOU KNOW?

Over the past 20 years, the Carnegie Mellon tech transfer team has assisted faculty and students with thousands of patent applications, licenses, options and other agreements. In 2022, Carnegie Mellon was ranked first in university technology transfer and commercialization by Heartland Forward, an economic development nonprofit. The group touted the university's unique entrepreneurial culture and focus.

LEARN MORE

NMR Pioneer Josef Dadok Dies at 98

Carnegie Mellon University Emeritus Professor Josef (“Joe”) Dadok passed away on Friday, Oct. 4, 2024, in Bloomington, Indiana, from complications of cancer. He was 98 years old.

Dadok was born in Detmarovice, Czechoslovakia, to Ferdinand and Barbora (Seberova) Dadok. A veteran and survivor of WWII, he became an electrical engineer, working in instrumentation at the Institute of Scientific Instruments of the Czechoslovak Academy of Sciences.

Dadok was referred to as the “founder of Nuclear Magnetic Resonance in Czechoslovakia.” He built the country’s first NMR spectrometers in the 1950s and 60s.

In 1967, Carnegie Mellon Professor Aksel Bothner-By invited him to serve as a visiting fellow at the university’s NMR facility. Dadok’s wife and two sons visited the U.S. in January 1968. While the family was traveling, the Soviet Union and other members of the Warsaw Pact invaded Czechoslovakia. The family stayed in the U.S., and Dadok became a full-time fellow at Carnegie Mellon.

Dadok continued his research at Carnegie Mellon, where he and Bothner-By constructed a multinuclear NMR spectrometer, equipped with a superconducting magnet operating at 250 MHz, in the late 1960s.

In 1976, Dadok was named technical director of the National NIH NMR Facility for Biomedical Studies at Carnegie Mellon. Bothner-By and Dadok collaborated with Intermagnetics General Corporation in 1976 to lead the team that built the first 600 MHz spectrometer. Housed at Carnegie Mellon, the 600 MHz spectrometer was the world’s most powerful system for many years and was used for leading-edge chemistry and biology research.

In 2013, the Central European Institute of Technology in Brno, Czech Republic, named its NMR center after Dadok. The Josef Dadok National NMR Centre focuses on using nuclear NMR to study the atomic structure of biologically significant molecules.

Dadok is survived by his sons, Jiri and Ludek, daughters-in-law Carolyn Begley and Debra (Beauchamp) Dadok, seven grandchildren and three greatgrandchildren. He is interred next to his wife, Marie (Janouskova) Dadok, at the Clear Creek Cemetery, Bloomington, Indiana.

Williams-Rolley Guides Chemistry Students to New Heights

In her free time, Lorna Williams-Rolley scales mountains. At work, she empowers graduate students to conquer their own academic peaks.

"I'm the one stop for grad students at any point in the program," said Williams-Rolley, the graduate program coordinator and academic program manager for Carnegie Mellon's Department of Chemistry. "I direct them where they need to go and see if I can help them solve their problems."

Williams-Rolley earned a bachelor's degree in chemistry from Grove City College in 2016 and began working in the Mellon College of Science in 2017. She earned her current position in 2018, and she said it was a good way to use her degree and experience in chemistry while helping others.

Williams-Rolley works with chemistry graduate students from application to graduation. She organizes recruiting visits for prospective students, connecting them with faculty and current students. Once admitted, she helps them find a research advisor and meet program requirements.

Along with offering advice, she helps plan graduation events and thesis defenses. She said she does her best to attend defenses so she can learn more about the students' experiences and accomplishments.

Bruce Armitage, professor and head of the Department of Chemistry, said her work helps the graduate student experience go smoothly.

"Lorna is the one constant in every student's experience here," Armitage said. "She is level-headed, discreet and shows excellent judgment."

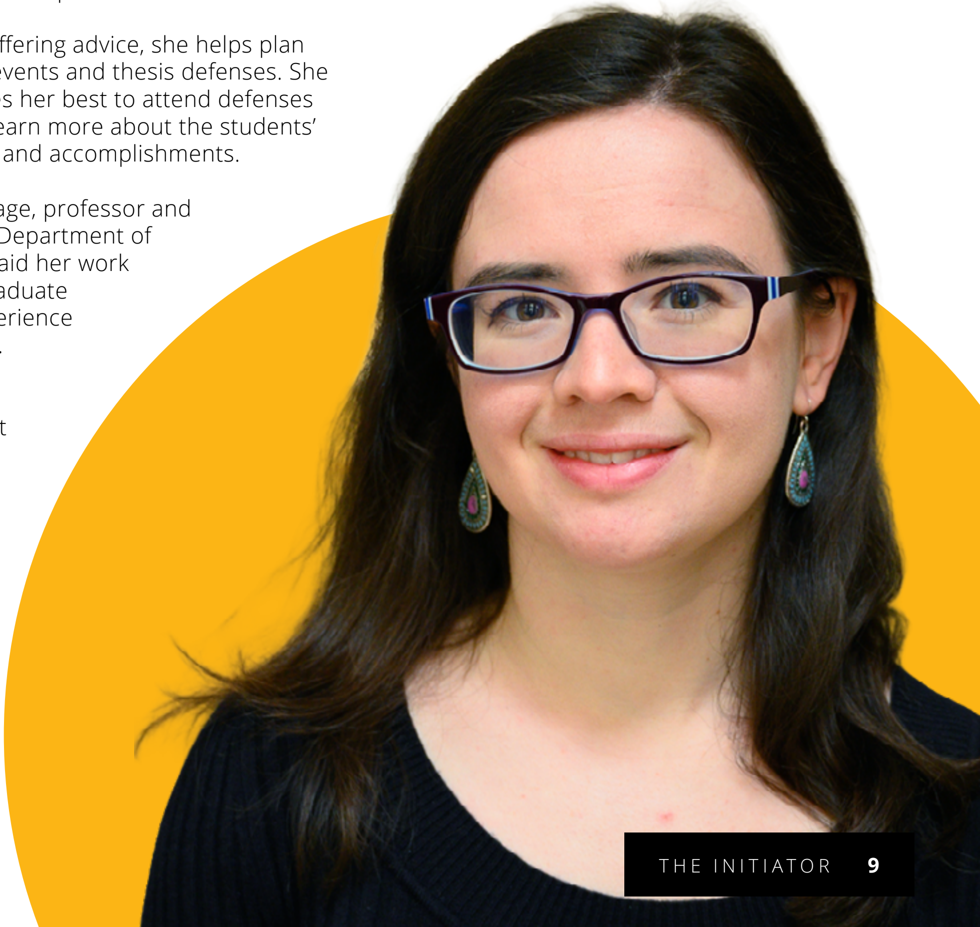
Williams-Rolley said one of the best parts of her work is seeing graduate students grow.

"I always enjoy interactions with students, especially because we have so many from across different countries," she said.

In her professional and personal life, Williams-Rolley embodies the spirit of a mountaineer. Just as she scaled Nevada's Mount Wheeler over spring break, her dedication to creating a supportive environment allows the students she works with to conquer their own summits.

"Lorna's love of the outdoors and the way she pursues challenges in her non-work life matches up perfectly with her ability to manage challenging things in her job," Armitage said. "Lorna is the bridge that brings everyone in the department together."

■ *Kirsten Heuring*



Research Roundup

Copper-Dependent Enzyme Catalyzes Unprecedented Reactions

A team of chemists from the University of California, Los Angeles, has discovered a new type of metal-containing enzyme from a natural fungus that can perform surprising halogenation reactions on organic molecules. The study, published in Nature, demonstrates for the first time that a copper-dependent enzyme can perform halogenation.

Carnegie Mellon University Associate Professor Yisong (Alex) Guo, whose research focuses on metal-containing enzymes, used electron paramagnetic resonance spectroscopy to confirm that the newly discovered enzyme contains two copper atoms at its active center.

This is the first known example of an enzyme using a copper center to perform halogenation.

In organic molecules, the halogenation reaction replaces a carbon-hydrogen bond with a carbon-halogen bond. It is a highly important synthetic transformation, particularly in the pharmaceutical industry. Functionalization of molecules with halogen substituents can dramatically improve their physical and pharmacological properties.

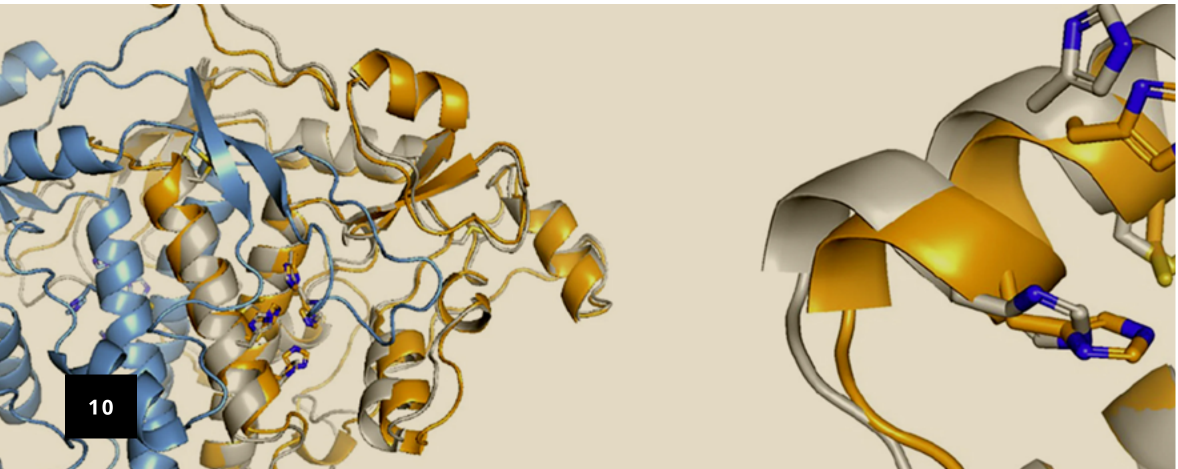
Nature has evolved enzymes called halogenases that perform halogenation reactions. Until now, the only enzyme family known to do these types of reactions involved enzymes with an iron center.

"Currently the prevalent idea is that if you want to perform C-H activation and a halogenation reaction, you should look to using an iron-based enzyme. My colleagues at UCLA have made a fundamental discovery that can potentially enrich our chemical toolbox with copper-based enzymes," Guo said.

The team from UCLA used multiple characterization techniques, including biochemical assays and mass spectrometry, to show that a protein previously labeled as "domain of unknown function (DUF) 3328" binds two copper atoms to catalyze the challenging halogenation reaction with high efficiency. They reached out to Guo for additional confirmation of the enzyme's potential structure at its metal center.

Using EPR, which is a method for studying molecules that have unpaired electrons, Guo concluded that the newly discovered halogenase contains two copper atoms at its center. The EPR results also suggested that the two copper atoms don't sense each other magnetically. Guo's spectroscopic results set up the initial entry point to further understand the detailed mechanism of this enzyme.

■ *Yi Tang*



Discovery of Crystallizable Organic Semiconductors with Machine Learning

Organic semiconductors represent a transformative technology that bridges traditional electronics with the versatility of organic materials. They make flexible, wearable devices and next-generation displays possible.

Crystallizable organic semiconductors (COS) represent a subset of organic electronic materials that have garnered substantial attention in recent years due to their unique properties and potential applications.

In collaboration with scientists at Princeton University, Carnegie Mellon University researchers Filipp Gusev and Olexandr Isayev, the Carl and Amy Jones Professor of Chemistry, devised a way to use machine learning (ML) to rapidly identify potential COS materials.

“This novel approach combines machine learning modeling of thermal properties of molecules with high throughput virtual screening,” said Gusev, a Ph.D. alumnus. “As a result, we identified three novel crystallizable molecules in platelet form. These three molecules build upon a pool of six that our collaborators at Princeton have seen previously to form platelets when fabricated through post-deposition annealing.”

Gusev is a first co-author on a paper titled “Discovery of Crystallizable Organic Semiconductors with Machine Learning,” published by the American Chemistry Society (ACS) in the Journal of the American Chemical Society. Gusev presented the work at the ACS Fall 2024 meeting in Denver, CO.

The team conducted a virtual screening of almost half a million commercially available molecules. Gusev built two ML models, one predicting melting temperature and a second predicting the enthalpy of melting. These two properties were important for narrowing down the pool of candidate COS materials by estimating a third key property: crystallization driving force. Together with a material’s melting point, crystallization driving force can act as a metric for anticipating crystal growth morphology — or resistance to thin film crystallization — in organic semiconductors. The ML model helped to prioritize a small number of candidates that collaborators at Princeton could efficiently experimentally analyze.

Gusev said that this project was one of the directions of his graduate work. He developed methods that combine ML with experiments.

“The whole idea of my research is to provide effective data-driven guidance for experiments across different disciplines,” Gusev said.

■ *Ann Lyon Ritchie*

Studying the Chemistry of Cloud Formation at CERN

Neil Donahue has long loved physics. He has focused his career, however, on concerns about the state of the environment. When he chose to train in meteorology and atmospheric chemistry, he thought he was leaving particle physics behind. "The irony is that here I am, doing particle physics at CERN," Donahue said, clarifying that the atmospheric particles he works with are much, much bigger than the elementary particles for which CERN is commonly known, like the Higgs boson.

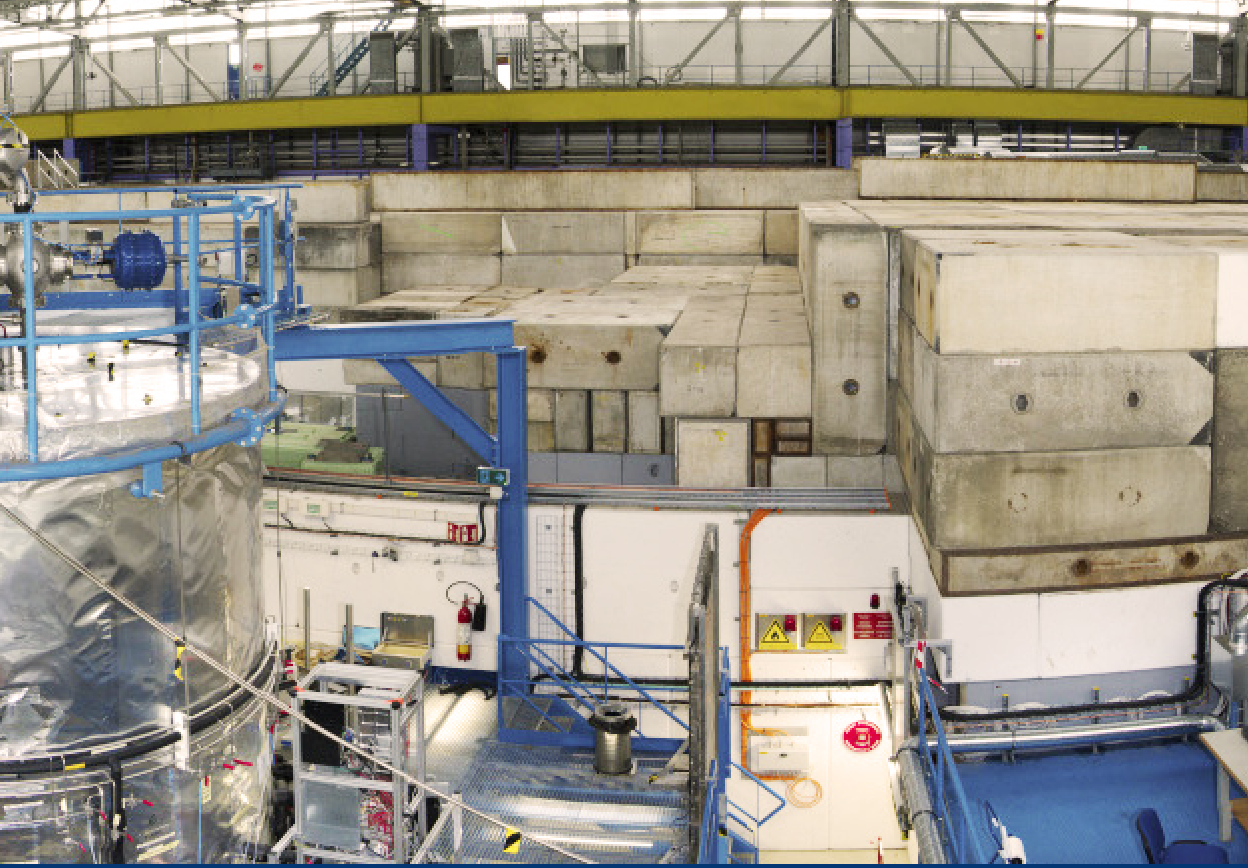
Donahue, Thomas Lord University Professor of chemistry, chemical engineering and engineering and public policy, is part of the Cosmics Leaving Outdoor Droplets (CLOUD) experiment at CERN. The goal of the interdisciplinary collaboration is to understand the chemistry and physics that lead to the formation of small molecular clusters that then grow into particles in the atmosphere.

The concentration of atmospheric particles affects the number of droplets in clouds. Clouds with more droplets are whiter. Whiter clouds reflect more solar radiation and can have a cooling effect on the planet, potentially masking some of the warming effect of greenhouse gases.

The connection between particles and clouds is one of the largest uncertainties left in our understanding of climate change.

"We need to understand what has happened since the preindustrial era and also be able to inform policy as we go forward," Donahue said. CLOUD scientists from 17 institutes in nine countries are establishing the experimental foundation to understand what clouds were like back in time, before scientists could measure them, and to predict what clouds will be like as climate changes due to human influence.

Recent CLOUD findings published in Nature show that the compound isoprene is driving particle formation in large regions of the tropical upper atmosphere. Prior to this work, scientists thought that isoprene was incapable of forming new particles in the atmosphere.



Isoprene is the most abundant non-methane hydrocarbon emitted into the atmosphere. It is released by trees, and the Amazon has some of the highest isoprene concentrations and the lowest sulfur dioxide concentrations over land. An accompanying paper reports aircraft observations made over the Amazon at the same time as the CLOUD experiments.

CLOUD combines fundamental experiments and modeling to study how particles form and grow from reactive gasses under atmospheric conditions. In the very cold and exceptionally clean conditions of the CLOUD chamber at CERN, researchers can set up the chemical mechanisms that generate gasses and then watch the gasses produce particles.

In new experiments, researchers studied particle formation from the oxidation of isoprene at -30 and -50 degrees Celsius. Donahue verified the observations by direct particle-phase measurements.

Donahue's core research interest is the way that organic compounds participate in making and growing a molecular cluster. Atmospheric particles form out of the air. One molecule sticks to another molecule, then another and another.

A cluster of molecules starts at about a nanometer in size and has to grow to about a hundred nanometers in order to affect clouds and climate.

Small molecules tend to be volatile, or not very sticky. Donahue is working to answer two closely-related questions: how sticky are organic compounds, especially to really small particles, and what was the chemistry that made the sticky molecules in the gas phase?

"The story of growth for particles, especially in the first one to 10 nanometers, is really important because most of them die," Donahue said.

The sticky molecules in organic compounds in the atmosphere don't come from emissions. They are created when a precursor molecule is oxidized in the atmosphere. Donahue is particularly interested in trying to understand that chemistry.

■ *Lauren Smith*

New ATRP Approach Could Transform the Manufacturing of Specialty Plastics

Researchers in Carnegie Mellon University's Department of Chemistry have improved a popular technology used to generate a diverse range of industrial plastics for applications from paints and coatings to adhesives and sealants. Using environmentally friendly reaction conditions, including running the reaction in water with light and a water-soluble dye, the novel method offers a promising approach for creating polymers in a greener and more practical way during the emulsion polymerization process.

In research published in the Journal of the American Chemical Society (JACS), chemistry doctoral student Xiaolei Hu developed a new method — light-driven miniemulsion atom transfer radical polymerization (ATRP) — that provides precise control over the resulting polymer structure.

"This is the first example of robust and efficient miniemulsion photoATRP under long-wavelength light, particularly red and near infrared lights," said Krzysztof Matyjaszewski, J.C. Warner University Professor of Natural Sciences.

ATRP allows scientists to string together monomers in a piece-by-piece fashion. By having precise control of polymer growth and shape, scientists can create highly tailored polymers with specific properties. Hu, a fourth-year doctoral student advised by Matyjaszewski, leverages photo-induced ATRP under longer-wavelength light so that it could be used more effectively in an emulsion.

He aimed to develop a greener ATRP reaction that can run under environmentally benign reaction conditions, such as in water, in open air and that can be initiated by a light source. Hu turned to longer wavelengths of light in the red and near-infrared regions of the spectrum. He used a common dye, methylene blue, as a photocatalyst.

In an earlier paper published in JACS, Hu found that this dye has photochemical properties that were applicable to ATRP. He demonstrated that methylene blue performed exceptionally well in a homogeneous solution in the open air, leading to rapid and well-controlled polymerization.

In the current work, Hu found that red/near-infrared light led to enhanced polymerization in a miniemulsion while UV light resulted in almost no polymerization. The scientists also showed that methylene blue, when exposed to red/near-infrared light, induces the rapid initiation of the ATRP process and provides control over polymerization.

"This finding is crucial for the practical application of photoinduced emulsion polymerization in a commercial setting," Hu said.

■ *Amy Pavlak Laird*

WE CAN
MAKE
A SCIENTIFIC REVOLUTION
POSSIBLE
together.

makepossible.cmu.edu/mcs
For more information on the
Mellon College of Science priorities,
please contact Lisa Iriguin
at lgeorgi@andrew.cmu.edu
or 412-268-2019.

MAKE
POSSIBLE

THE CAMPAIGN FOR
CARNEGIE MELLON UNIVERSITY

RESEARCH FEATURE

Chemistry's Pollution Blind Spot: How CMU Researchers Are Filling the Gaps

by Heidi Opdyke

Everyday items like carpets, shower curtains, cosmetics and even food can have harmful chemicals hidden inside that can lead to long-term health effects.

The number of synthetic chemicals and products being used and produced that can contaminate the environment during their lifecycle has risen dramatically over the past 30 years. This includes compounds such as halogenated flame retardants, polymers and per/polyfluoroalkyl substances (PFASs), also known as “forever chemicals” because they persist in the environment and human body.

“The old viewpoint of pollution is that it’s coming from external sources, like a factory or a powerplant, but it’s also coming from the flame retardants in my cellphone that I touch hundreds of times a day,” said Ryan Sullivan, associate director of Carnegie Mellon University’s Institute for Green Science and a professor of chemistry and mechanical engineering. “We really want to do a much better job of reducing the amount of harmful chemicals that get into the environment, into organisms and into humans that cause health damage. The best way to do so is by not making chemicals that are too persistent or toxic in the first place.”

Some of the pharmaceuticals, PFASs and other chemicals can transform into even more problematic compounds, but it is hard to identify these transformation products using standard approaches. Sullivan, Carrie McDonough, associate professor of chemistry; Olexandr Isayev, the Carl & Amy Jones Professor of Interdisciplinary Science; and Ana Torres, assistant professor of chemical engineering, are working to change that.

THE RISE OF SYNTHETIC CHEMICALS

More than 10,000 synthetic chemicals are used to make plastic products, and hundreds of thousands of chemicals are used in other industries, Sullivan said.

Advancing sustainable chemistry requires the capability to predict what changes chemicals may undergo and what happens to the resulting transformational products. Sustainable chemistry also promotes the use of chemicals and synthetic methods that reduce energy needs, are more efficient, have reduced costs and avoid generating harmful environmental pollutants, thus reducing the cost of harmful health effects and lost lives.

Sullivan is the primary investigator on this initiative. Sullivan, along with McDonough, Isayev and Torres, are developing high-throughput experimental and computational methods that acquire the chemical data needed to inform environmental molecular lifecycles.

The researchers said that these environmental and biological chemical reaction networks will screen for transformation products that are likely persistent or prone to bioaccumulation. This more rapid chemicals analysis will then guide sustainable chemical assessment such that likely harmful chemicals can be identified much earlier in their development lifecycle.

“Our big focus is to assess the ability to predict the fate of a molecule under environmental and biological conditions. What does it turn into? And where does it go?” Sullivan said.

Sullivan said that by understanding how molecules can transform and how quickly under different conditions, the data can inform how long they’ll exist in the environment.

“It’s an understudied — but important — topic,” he said. “We need to work to connect the world of environmental chemistry and what we know and how we use that information to better evaluate and design chemicals and materials that are more sustainable in nature.”

UNVEILING END OF LIFECYCLE FACTS

Current analyses generally focus on the earlier portion of the lifecycle of molecules, such as the extraction of resources, manufacturing and distribution of products. Sullivan said that the work doesn’t account for damages caused at the end stages of the lifecycle during use and then after disposal.

“This is a huge blind spot,” Sullivan said. “And it gets to the heart of the problem with plastic pollution. All the damage caused by forever waste is never factored into the price that we pay or what a store pays to buy plastic bags.”

Torres will provide expertise on how to advance lifecycle analysis applied to evaluate chemical alternatives and their sustainability. In particular, she will focus on the later life stages for during and end of use that are usually neglected due to the lack of needed data to estimate these costs.

McDonough said that Carnegie Mellon is uniquely equipped to tackle this problem.

“We’re very strong in computational chemistry and one of the few U.S. universities with a chemistry department that focuses on environmental chemistry, so it’s an ideal mixture of experts,” said McDonough, who studies how PFASs accumulate in organisms and brings expertise in environmental chemistry and bioanalytical techniques. For this work, she will focus on developing and evaluating experimental approaches to determine chemical properties that describe bioaccumulation potential and identify biological transformation products.

“Add in our automated science initiative, high throughput capabilities and libraries of compounds for testing, and we’re well positioned to learn how molecular structure can predict downstream environmental and health impacts,” she said.

“Our big focus is to assess the ability to predict the fate of a molecule under environmental and biological conditions. What does it turn into? And where does it go?”

The scope of the work is large, and the combined experimental and computational high-throughput analysis will allow them to evaluate many chemicals more quickly. The team is working to identify ways to support a postdoctoral researcher and several graduate students.

BIG DATA ON MINISCULE MOLECULES

The collaborators are expecting to work with a massive volume of data.

“We use machine learning to guide high-throughput experiments and scale the amount of experimental data that we can obtain,” said Isayev, a member of the Department of Chemistry with a joint appointment in the Department of Materials Science and Engineering and is affiliated with the Department of Computational Biology.

Isayev, Sullivan and McDonough are involved with Carnegie Mellon’s automated science initiative, which is developing the future of autonomous laboratories. Gabe Gomes, an assistant professor in the Departments of Chemistry and Chemical Engineering, and students already have demonstrated that AI systems can autonomously plan, design and execute within minutes a chemical reaction so complex it earned its human inventors a Nobel Prize in 2010.

A major challenge that the team’s high-throughput methods will address is reducing the time and effort required to measure or predict all the environmental chemical properties for each chemical and its persistent transformation products.

Isayev’s group brings data-driven methods to accelerate simulations to support creating more effective and efficient simulations. The collaboration on sustainability expands on work from Isayev’s group.

“We’ve done drug discovery to predict molecular behavior, and the physics for this work is similar but with slightly different applications,” Isayev said. “Our experience will help us predict bioaccumulation of chemicals in various organisms, sediment, soils, water and plants.”

For this work, Isayev is focusing on developing and evaluating the new computational approaches to predict environmental chemical properties from structure. He also is leading the development of chemical reaction networks that will consolidate data from experiments, computational analysis and literature.

BUILDING A GLOBAL RESOURCE FOR SAFER CHEMISTRY

With the information collected, the researchers aim to build a library to share the methods and data including predictions about the environmental impact and sustainability of chemicals to help inform regulatory agencies, public health experts and other researchers.

The combined experimental and computational data will be used to predict the ‘environmental molecular lifecycle’ of a given chemical, which provides essential information to evaluate the sustainability and hazards of any chemical much earlier in its development lifecycle, reducing barriers in inventing safe and sustainable chemicals.

Student & Postdoc Stories

Martin Earns Hugh D. Young Graduate Student Teaching Award

Organic Chemistry courses tend to have a bad reputation. Colin Martin was determined to flip the script.

“Students come in with a preconceived notion of what it’s going to be like, and it feels really good to just smash that the moment they walk in and hopefully change their mind whenever they leave,” said Martin, a fifth-year Ph.D. student in the Department of Chemistry.

He set a high bar for himself, and he cleared it.

“Thank you for making me like orgo,” wrote one of his students. “I never thought I would be able to say that.”

Mellon College of Science students and faculty recognized his excellence in teaching by awarding him this year’s Hugh D. Young Graduate Student Teaching Award.

Martin has been a teaching assistant for several semesters of Organic Chemistry I and II as well as Modern Chemistry. Even though these are some of the largest and most demanding courses, Martin earned exceptionally high TA evaluations.

Students appreciated that Martin was interested in learning about them as people and creating a supportive environment where they felt encouraged to engage actively in the material.

In the Armitage lab, Martin conducts research related to peptide nucleic acid synthesis and its applications to human disease therapies. He anticipates wrapping up his Ph.D. work and defending his thesis in the next few months. After graduation, he plans to use his teaching skills in a different environment — as a patent agent for a law firm. Patent agents bring a technical background to the patent process, enabling them to grasp the complex ideas generated by inventors.

“I feel like I have this ability to explain complex topics to a broad audience, and I’ll be able to leverage that experience in what will be my job as a patent agent,” Martin said. “I’m really excited about it.”

■ *Amy Pavlak Laird*

Koby Earns Biophysical Society Student Research Achievement Award and NIH Fellowship

Ben Koby computes new ways to develop potential drug candidate molecules. When the Critical Assessment of Computational Hit-Finding Experiments (CACHE) Drug Discovery Challenge #1 was announced, he was excited to participate.

Teams were tasked with using computational methods to find hits, potential drug targets, for leucine-rich repeat kinase 2 (LRRK2), a donut-shaped protein implicated in familial Parkinson's disease. Because of its shape, researchers face difficulties finding molecules that bind to LRRK2.

"The goal of the competition was to find novel, small molecules that bind to an orphan drug target," said Koby, a Ph.D. student in the Department of Chemistry. "The protein itself is the most common genetic cause of familial Parkinson's disease."

Koby was part of the Carnegie Mellon CACHE team, which developed an active learning cycle workflow with automatic machine learning based on absolute free binding energy simulations to predict how molecules would interact with LRRK2. They then performed the simulations on the Pittsburgh Supercomputing Center's Bridges-2 supercomputer. Out of 800 molecules simulated, they chose 76 for experimental validation and found five that bind to LRRK2. In the second round of the competition, the team identified another eight experimentally active compounds based on their previous results.

CACHE was created to find the most efficient computational methods for initial hit-finding. In the first challenge, the Carnegie Mellon team tied for first place.

Koby presented his work at the Biophysical Society's Annual Meeting in February. He earned a Student Research Achievement Award for his outstanding presentation during the poster competition.

Koby's work also was recognized by the National Institutes of Health (NIH). He earned the Ruth L. Kirschstein Predoctoral Individual National Research Service Award Fellowship, which funds doctoral students' dissertations and provides mentored research training. Koby will use the award to develop free energy-based multi-objective active learning machine learning methods. These methods will optimize compounds to make them bind more effectively for a single target or multiple targets.

"As a scientist, it always feels good to have recognition for what you've done," Koby said.

■ *Kirsten Heuring*

Doctoral Fellowships

NICOLE AUVIL

Kwolek Fellowship

Nicole Auvil builds mass spectrometry instrumentation and methods to make improved mass-to-charge measurements. Working with Research Professor Mark Bier, she developed an ultrasharp needle that emits a corona discharge, which ionizes the ambient air — and whatever molecules it may contain — in a small region around the needle tip for mass-to-charge analysis and detection. The needle is housed inside what Auvil and Bier refer to as the "super-sniffer," which they have used to analyze many sample types — medicine, air pollution, receipt paper coatings and a sample of residue from a 2,500-year-old bronze cup used to hold incense.

XIAOLEI HU

John and Nancy Harrison Legacy Fellowship

Xiaolei Hu is pioneering new techniques to create eco-friendly polymers used in industrial applications such as paints, coatings, adhesives and sealants. Hu's novel approach to improve the emulsion polymerization process relies on environmentally conscious reaction conditions, including the use of light, water and a water-soluble dye, offering a promising pathway to greener polymer production. Hu also has contributed new ways to modify nucleic acids like RNA with polymers. Notably, he pioneered a method using methylene blue as a photocatalyst activated by near-infrared light, enabling polymerization in a high-throughput manner at ambient conditions.

LIANSHUN (EVAN) LUO

McWilliams Fellowship

Lianshun (Evan) Luo creates atomically precise nanoclusters of only dozens of gold atoms that have unique electrical, magnetic and optical properties. Since joining Chemistry Professor Rongchao Jin's group, Luo has been synthesizing gold nanoclusters with a specific optical property — emitting light in the near-infrared regions of the electromagnetic spectrum. Luo developed a method to synthesize a series of rod-shaped gold nanoclusters that absorb and emit in the near-infrared, making them 100 times stronger than commercially available organic dyes. The work highlights the quantum rods' promise for use in biomedical imaging applications, including deep, non-invasive imaging and image-guided cancer surgery.

Learn more about MCS Fellowships: https://www.cmu.edu/chemistry/grad/fellowships/index.html

The Chemger Games

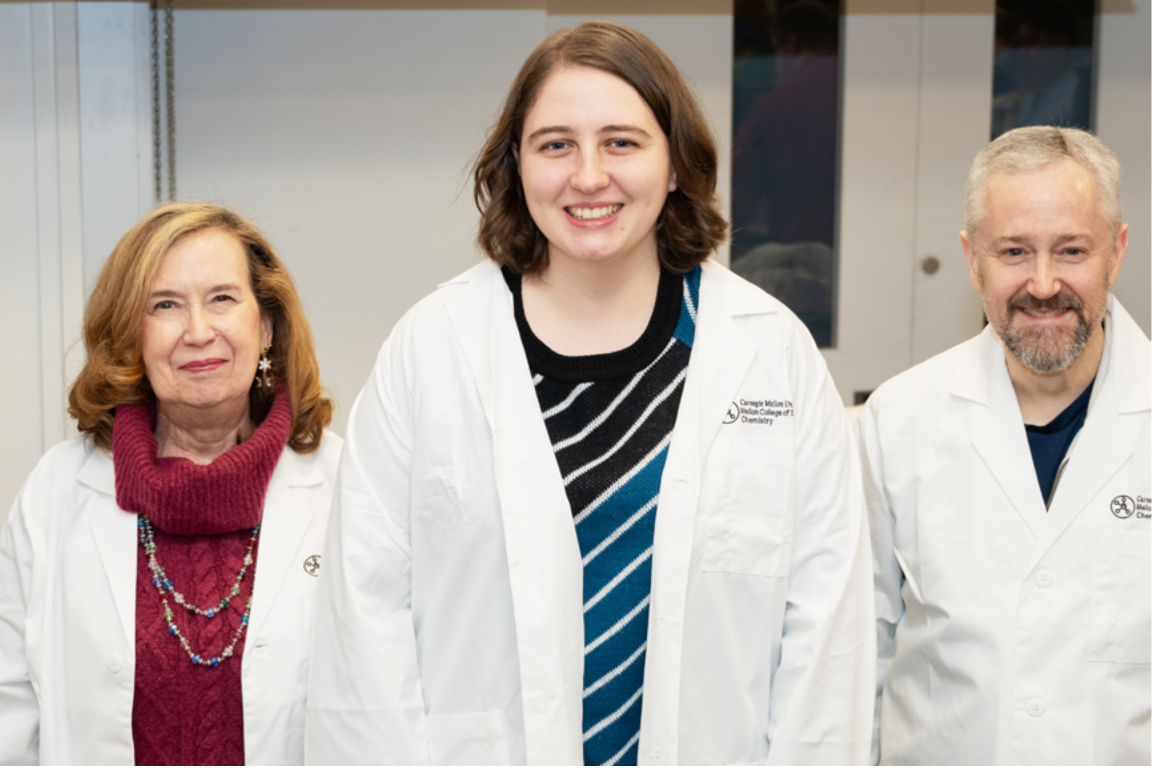
For one night only, the Department of Chemistry transformed the Mellon Institute into an escape room. Participants explored labs, used their chemistry knowledge to solve puzzles and met fellow undergraduate and graduate students. Sydney Prescott, Stella Trickett, Iris Reed, Jessica Wei and Jacob Kadir won the fall 2024 edition.

SHU AWARDED GOLDWATER SCHOLARSHIP

Sheng Shu, a rising senior majoring in chemistry and computer science, was selected to receive a Barry Goldwater Scholarship in 2025. Shu's fascination with chemistry is rooted in curiosity about the fundamental aspects of the natural world. Over time, that interest grew to include computer science, which offered new tools for examining chemical systems. One of Shu's personal milestones in the lab has been a defining moment in his education so far: building and testing a model that could generate de novo molecules — molecules designed and generated from scratch.

"It was the first bridge I built myself between the two fields," he said.

His current research focuses on molecular representation, developing a model that encodes molecules into a fixed number of values.



Prescott Develops Chemicals and Musicals

When she was in high school, Sydney Prescott learned about the Department of Chemistry's annual student-produced murder-mystery musical dinner.

"This program showed that people cared so much that they were willing to do something so elaborate for fun," she said. "I realized this would be a good place for me."

Prescott recently graduated with majors in chemistry and environmental & sustainability studies and she worked with about 15 other students to produce this year's dinner, which was themed to the musical "Chicago."

The production, a CMU tradition for almost 20 years, provides a bonding experience for those involved and a way for them to share their skills outside of the classroom.

"I've really enjoyed working on different teams, no matter what the activity or opportunity has been," she said. "For something like the murder-mystery dinner, I've seen how everyone has to come together and figure out each other's strengths to work toward the end goal of the final performance."

Prescott worked for three years as an undergraduate researcher in the lab of Chemistry Professor Stefan Bernhard. She synthesized iridium-centered complexes and tested their luminescent properties and potential applications in renewable energy systems.

"I've had to adjust the synthetic method to improve the yield and purity," she said. "It's been a lot of work at the bench, doing chemistry."

She credits Karen Stump, teaching professor and director of undergraduate programs in the Department of Chemistry, with helping her find opportunities. Aided by chemistry doctoral student Mitch Baumer, she learned how to contribute to the lab's research and completed a project funded by a Summer Undergraduate Research Fellowship.

This fall, Prescott will begin a Ph.D. in chemistry at the University of Rochester

"I feel a lot more prepared for the next step. I want to be able to have leadership over the experiments I'm running," she said. "Whatever my future goal is, I want to have a really solid understanding of research and be able to make informed decisions about what direction the project goes in."

■ *Stacey Federoff*

LAB COAT CEREMONY

At the inaugural lab coat ceremony, students donned coats to mark their official entry as majors in the Department of Chemistry.

Above: Karen Stump and Bruce Armitage help Amber Chang into a lab at the Nov. 14, 2024, ceremony.

Alumni News

Innovator Uses CMU Education To Combat Rare Diseases

Carnegie Mellon University alumnus Jeff Milton has his eye on the horizon in more ways than one.

An avid pilot who flies vintage military aircraft and other planes, he also is looking for ways to provide new therapies to patients with rare diseases.

According to the U.S. Government Accountability Office, only 5% of the nearly 10,000 identified rare diseases have Food and Drug Administration-approved treatments.

As co-founder for the drug discovery company La Jolla Labs, Milton is on a mission to find RNA therapeutics to address rare and complex diseases through a combination of artificial intelligence, next-generation sequences and RNA biology.

“Pharmaceutical companies often neglect these diseases due to high costs related to research and development for a small market,” he said. But La Jolla’s screening technology reduces costs and time for patients.

La Jolla uses RNA as a platform because it plays a crucial role in various cellular processes, and many of the rare diseases come down to specific molecules that need to be targeted.

“We target RNA because it contains a human’s genetic makeup and it contains the mutations. We can target those specific mutations at the genetic level. Every therapy is genetically focused down to the nucleotide,” he said.

His Carnegie Mellon education is helping him create to support patients and their medical teams.

“I wanted fundamental knowledge of life, and chemistry was my focus. I spent so much time in the Mellon Institute at all levels,” said Milton, who graduated from Carnegie Mellon in 2004 with a bachelor’s degree in chemistry. “Faculty were so open to exploring and supporting what I wanted to do that they thought was novel and interesting.” He said the entrepreneurial and coaching opportunities available at Carnegie Mellon today are stronger than they’ve ever been.

Among the professors Milton interacted with was Krzysztof Matyjaszewski, J.C. Warner University Professor of Natural Sciences and director of the Center for Macromolecular Engineering. Milton was visiting his lab when he first heard of atom transfer radical polymerization (ATRP), a novel method of polymer synthesis that revolutionized the way macromolecules are made.

“Every day I dive into science and technology that I can directly link to the skills I learned at Carnegie Mellon,” Milton said.

Milton also worked with David Yaron, who recruited Milton to design the first Department of Chemistry website. It’s when Milton first started developing software writing skills. Among the projects that Milton worked on with Yaron was Chem Collective, the precursor to Real Chem, courseware for introductory chemistry classes that marries in-person instruction with online instruction and practice.

Prior to co-founding La Jolla Labs, Milton served as senior director and head of data science at Arcturus Therapeutics, where he led the development and implementation of data-driven strategies for mRNA therapeutics. Additionally, he served as director and associate director at Ionis Pharmaceuticals.

He also is an executive fellow at St. Jude Children’s Research Hospital in Memphis, where he is helping to optimize rare disease therapies. He is hoping Carnegie Mellon might aid that effort.

“Every day I dive into science and technology that I can directly link to the skills I learned at Carnegie Mellon.”

“I’ve been talking to the Department of Chemistry, and Department Head Bruce Armitage, specifically, about building a research-grade synthesis lab to make the compounds needed,” he said. “It’s one thing I’m super excited about, and I think it would be great for Carnegie Mellon and the Mellon College of Science.”

Milton, who was a student-athlete on the Men’s Swimming and Diving team, is now giving back to the place that gave him so much as a member of the Mellon College of Science Dean’s Council.

“CMU defined my life. It made me who I am. I had support from research faculty who saw my passion and drive,” he said. “I’m going to dedicate a significant portion of the second half of my life to CMU to help make sure others receive that same support.”

■ *Heidi Opdyke*

Tartans on the Rise

THE BEAUTY OF INNOVATION

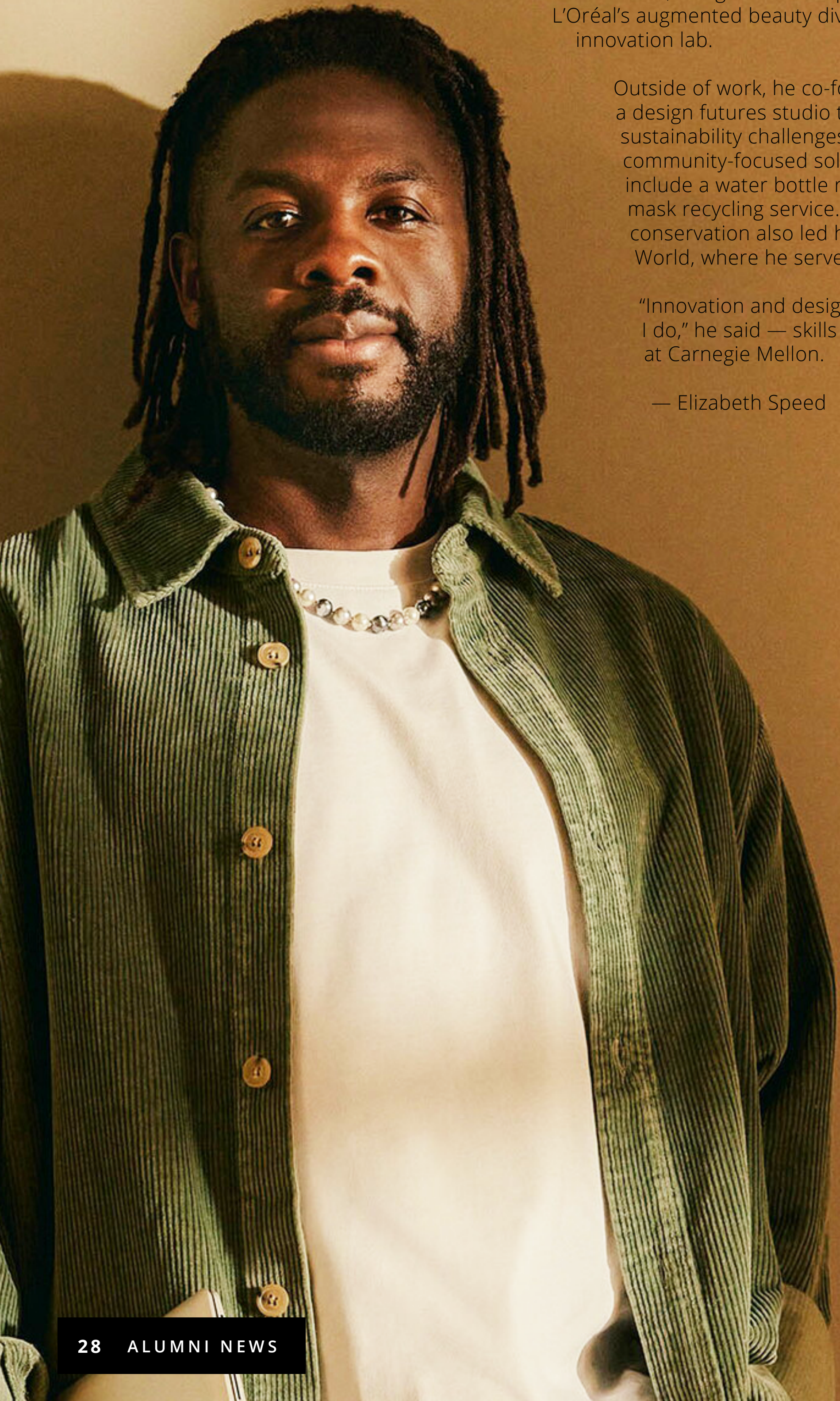
Dominic Akerele is shaping the future of beauty tech at L'Oréal Groupe, where he's helped develop innovations like smartphone-applied blemish coverup, personalized skin serums and the Water Saver salon showerhead — named one of Time's best inventions of 2021.

A 2015 chemistry grad from Carnegie Mellon, Akerele blends science, design and entrepreneurship in L'Oréal's augmented beauty division, a global innovation lab.

Outside of work, he co-founded Waterboys, a design futures studio tackling urban sustainability challenges through local, community-focused solutions. Projects include a water bottle rental system and mask recycling service. His passion for water conservation also led him to One Young World, where he serves as an ambassador.

"Innovation and design connect everything I do," he said — skills he credits to his time at Carnegie Mellon.

— Elizabeth Speed



COMPOSING MUSICALS WITH A MESSAGE

Alex Petti has something to say … or rather, something to sing. He's a composer, lyricist and guitarist achieving his musical theater dreams in New York City.

Along with classmate and CFA alumna Annie Pulsipher, he debuted "The Trouble with Dead Boyfriends" in 2023, a project they started together at Carnegie Mellon as part of the PLAYGROUND festival of student work. Packed with wordplay and puns and driven by a pop-punk score, it's the story of three best friends dreaming of perfect prom dates who end up with literal monsters.

Petti, who graduated in 2015 with a bachelor's degree of science and arts in chemistry and music composition, is working on several new projects.

"CMU's BXA program gave me the tools to be able to pursue music," Petti said.

"Studying chemistry in the Mellon College of Science developed the analytical side needed to manage everything that goes into producing a musical, and extracurriculars like Scotch'n'Soda developed leadership skills."

— Elizabeth Speed


Link-Belt
Link-Belt
Link-Belt
PEPPER SPACE
8065

A Sustainable Future

When the Richard King Mellon Hall of Sciences opens in 2027, faculty from the Department of Chemistry will be among the new residents.

Department Head Bruce Armitage said the departmental plan is to bring together computational chemistry, environmental chemistry and chemical biology to advance efforts in sustainability.

“Sustainability is a theme that runs through everything we do,” Armitage said. “We value chemistry with a conscience.”

That theme not only draws on research and student preparedness but also in the department’s operations.

Several areas of sustainability are included in the new building’s design. To help maintain energy efficiency, the building will include high-performance glazing, LED lighting and low-flow plumbing fixtures, as well as chillers, beams, boilers and energy recovery systems designed to further minimize energy usage.

A green roof will help capture stormwater and provide additional building shading and insulation. Native plant species and water management features will be integrated into the landscaping. The building will also include bicycle facilities and electric vehicle charging stations to support more-sustainable methods of transportation.

“The new space represents more than just a change of address — it’s a commitment to a more sustainable future,” Armitage said. “With cutting-edge research, environmentally conscious design and a focus on preparing the next generation of scientists, the department is poised to lead by example in shaping a greener, more responsible world through chemistry.”

For more information on the Richard King Mellon Hall of Sciences, please visit: cmu.edu/hall-of-sciences

To make your gift, please contact:
Jenny Belardi, Chief Advancement Officer
jbelardi@andrew.cmu.edu · 412-268-8810

Carnegie Mellon University
Mellon College of Science
Chemistry

5000 Forbes Avenue
Pittsburgh, PA 15213

@cmuchemistry

@CMU_Chem

@cmu_chem

Website: **www.cmu.edu/chemistry**

Online Magazine: **magazine.mcs.cmu.edu/chemistry**