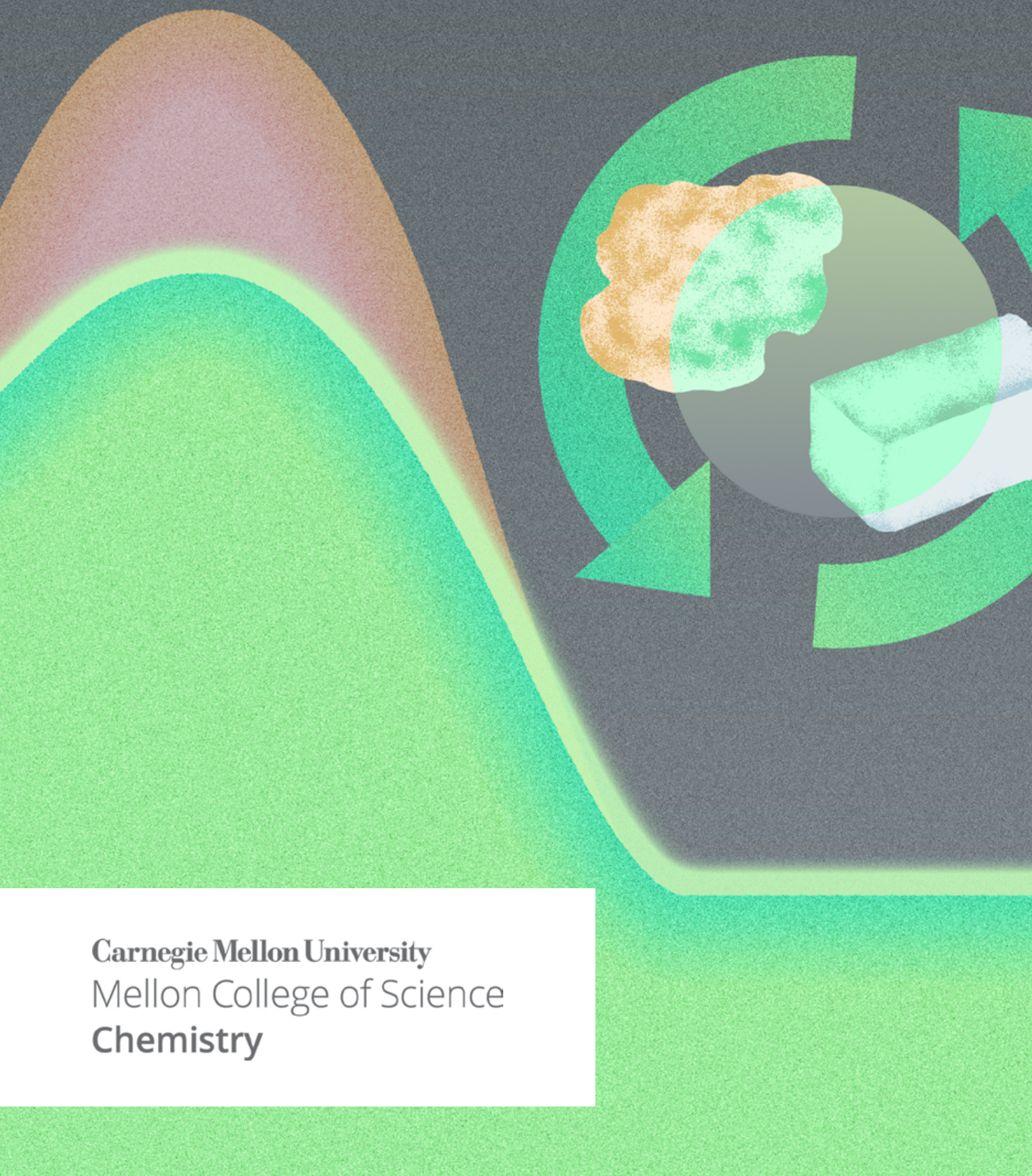
2024

THE INITIATOR



Carnegie Mellon University
Mellon College of Science
Chemistry

THE INITIATOR

The Department of Chemistry

The Initiator is published yearly by the 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.

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Letter from the Department Head

Greetings CMU Chemistry Alums and Friends! We're delighted to bring you this year's issue of The Initiator, which is packed full of exciting and inspirational stories about our research and educational endeavors. The article about Gabe Gomes' development of Coscientist, a software tool that facilitates the design and execution of experiments in a remote, automated lab, represents in microcosm the department's commitment to integrating experimental, computational and automated science throughout our curriculum and research program. Meanwhile, the research feature on Isaac Garcia-Bosch's work highlights our department's strength in catalysis, an essential cog in our world-leading program in environmental and sustainable chemistry.

Our students — undergraduate and graduate — are the lifeblood of the department. They do so much of the research, serve as teaching assistants and mentors, host outreach activities and organize symposia at scientific meetings. They even run in the Olympic Marathon trials! All of the students and alumni featured are compelling, but among the standouts are Ananya Kapur, who translated her CMU experiences into a cosmetics company, and the husband-and-wife team of Raman Bahal and Anisha Gupta, whose story reflects hard work, curiosity, love and family.

I want to highlight some important leadership changes. Professor Kevin Noonan is our first associate department head and will be invaluable to day-to-day operations. Professor Gizelle Sherwood added director of undergraduate studies to her title of director of laboratories. Gizelle assumed this responsibility from Professor Karen Stump. Karen, this year's winner of the Richard Moore Education Award for substantial and sustained contributions in MCS, will retire in 2025. Expect to see much more about Karen's transformative impact in next year's issue of The Initiator.

I also want to update you on a fund that supports graduate students who mentor undergraduate research. Earlier this year, Dr. Bruce Gelin (BS 1967) made a generous gift to support awards to four outstanding graduate students: Kaizheng Liu (Kietrys Lab), Sunipa Goswami (Garcia-Bosch Lab), Riley Weatherholt (Sullivan Lab) and Xiaowei Ma (Collins Lab). We would be delighted to receive additional donations to this fund. I am also pleased to announce a new giving opportunity to permanently endow the Pople Lectureship, which brings top scientists and important visibility to the department.

The next year promises to be an exciting one. We broke ground on the new Richard King Mellon Hall of Sciences during Carnival weekend. "RKM" will become the home for several of our research groups when it opens in late 2027. Meanwhile, the CMU Cloud Lab is in a soft-launch phase with faculty and students testing instruments. We anticipate using this one-of-a-kind academic facility in upcoming courses and research projects.

It was great seeing many of you at our Spring Carnival event, and I hope to see many more in Pittsburgh or during my upcoming travels. (See the back page about requesting an alumni dinner!) Follow us on social media (@CMU_Chem) to keep up with the latest news and remember, you will always have a home with us.

Bruce Armitage
Professor and Head
Department of Chemistry
army@cmu.edu

Faculty Notes

Pople Lecture Returns

John A. Pople's groundbreaking contributions to elevate quantum chemistry won him a joint 1998 Nobel Prize.

Pople, the former J.C. Warner Professor of the Natural Sciences, was affiliated with the Mellon Institute and Carnegie Mellon University for more than 30 years. During this time, his work was integral to launching quantum chemistry, especially *ab initio* electronic structure methods, as a powerful and now pervasive means for predicting and interpreting the structure and properties of molecules.

Applications of quantum chemistry are found in areas as diverse as drug design, materials science, chemical reaction theory and computational spectroscopy.

"One of Pople's key contributions is the development of a systematic computational framework that enables efficient quantum chemistry calculations at different levels of accuracy or theory," said Professor Hyung Kim, who led efforts to revive the John A. Pople Lecture in Theoretical and Computational Chemistry, a biennial event hosted by the Department of Chemistry that celebrates work in quantum chemistry.

"This revolutionized the field of quantum chemistry because researchers — not only in quantum chemistry but also in other fields — can use Pople's methods to study and understand molecular systems," Kim said.

Molecular systems — and the electrons that inhabit them — require extremely complicated numerical calculations to understand their electronic properties. Professor Krishnan Raghavachari of Indiana University, one of Pople's students, is well-known for his work on electron correlation methods and is a pioneer in the development of fragmentation-based methods in quantum chemistry that enable quantitatively accurate studies on large molecules. He has expanded his research profile in recent years to include machine learning in quantum chemistry, and computer-aided design of novel functional materials. Raghavachari will deliver the next Pople Lecture on Oct. 9, 2024.

"John Pople's work had incredible impact on quantum chemistry, and everything he did was most fundamental as well as highly applicable. The lesson I learned from him was to do impactful work that can influence a broad range of scientists," Raghavachari said.

Originally from India, Raghavachari received his Ph.D. from Carnegie Mellon in 1981. He joined Bell Laboratories as a research scientist in 1981 and later received the Distinguished Researcher Award in 1987. He joined Indiana University as a Professor of Chemistry in 2002 and was appointed as a Distinguished Professor in 2014.

■ *Heidi Opdyke*

Scan to contribute to the John A. Pople Lecture Fund

SAVE THE DATE

John A. Pople Lecture in Theoretical and Computational Chemistry

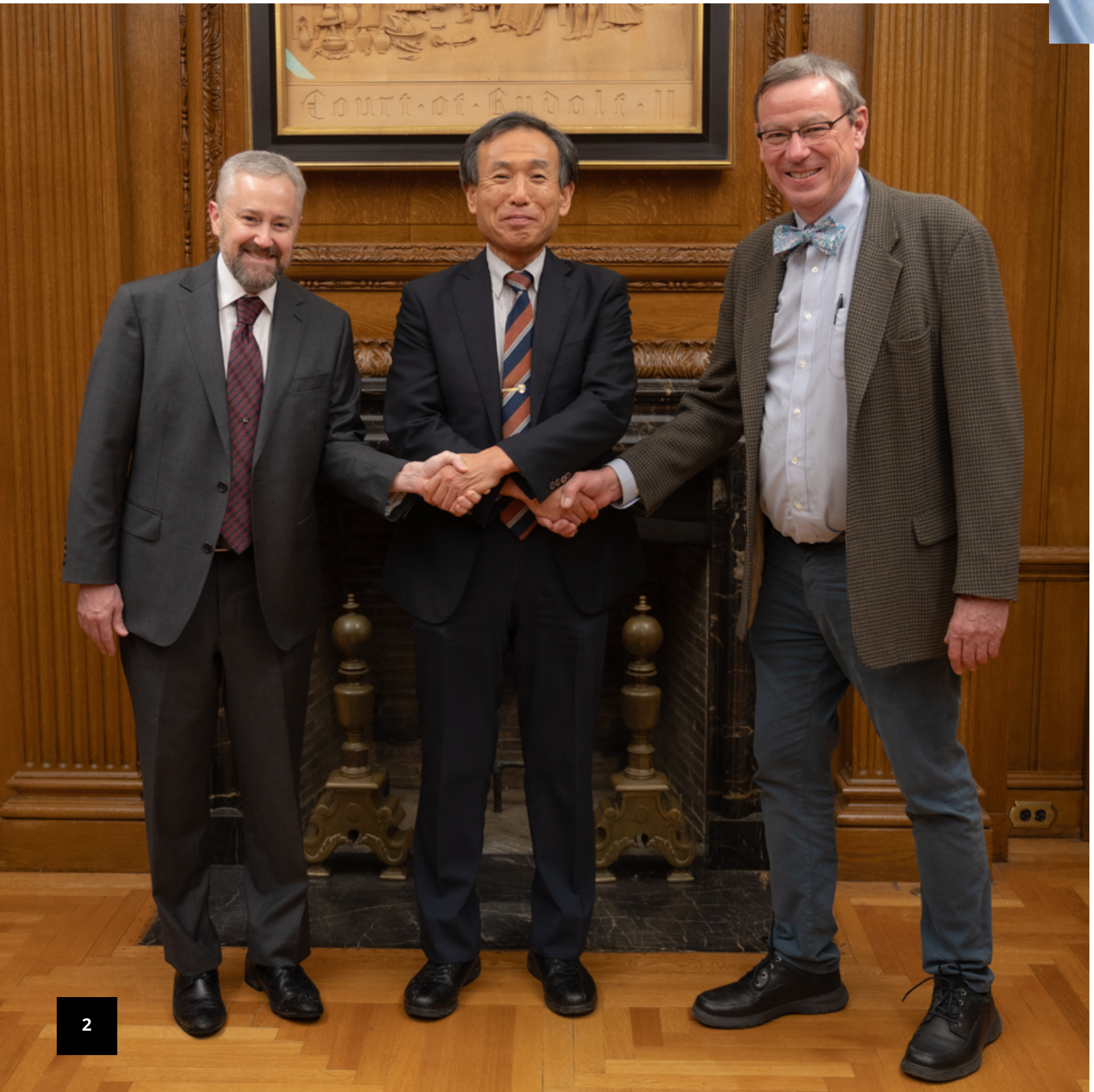
Krishnan Raghavachari

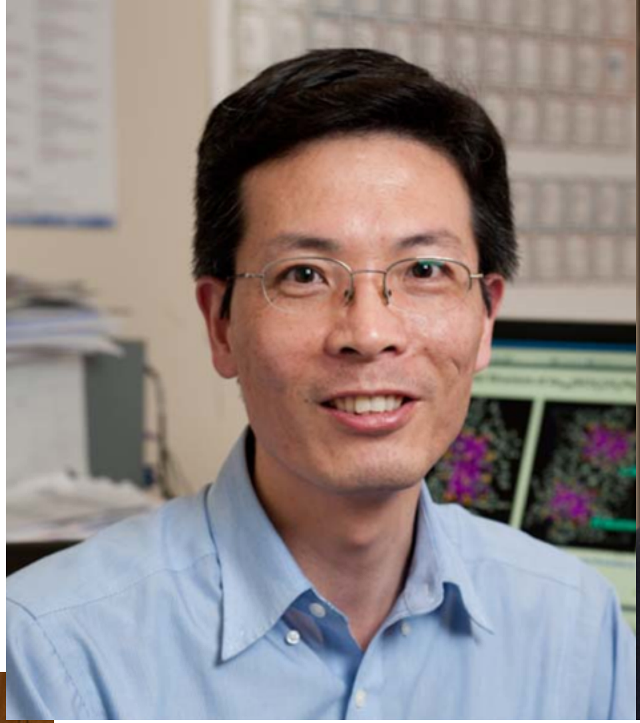
4 p.m., Wednesday, Oct. 9
Mellon Auditorium, Mellon Institute

CMU, Konan To Collaborate on Nucleic Acid Research

Carnegie Mellon University and Konan University have signed a formal Agreement for Academic Exchanges and Collaborations. This new partnership will connect CMU's Center for Nucleic Acids Science and Technology (CNAST) with Konan's Frontier Institute for Biomolecular Engineering Research (FIBER), which share expertise in the chemistry and biology of nucleic acids such as the natural versions (DNA and RNA) as well as synthetic analogues known as peptide nucleic acids (PNA). FIBER Director Naoki Sugimoto visited CMU Jan. 18 – 19, 2024, to meet with upper administration officials, faculty and students and deliver a public seminar on his research. CNAST Co-director and Chemistry Department Head Bruce Armitage visited Konan in turn, for a signing ceremony, scientific discussions and a public seminar.

■ *Heidi Opdyke*





Two Chemistry Faculty Named Among World's Most Highly Cited Researchers

Two researchers from Carnegie Mellon University's Mellon College of Science are part of the 2023 Highly Cited Researchers list by Clarivate Analytics.

Rongchao Jin, professor of chemistry, was listed among the most cited researchers in the field of chemistry. Jin's research focuses on nanochemistry, and he is well known for developing new methodologies to create gold nanoparticles with precise numbers of atoms. He and his students have continuously pushed this work forward, refining gold nanoparticles so they can be used to create functional nanomaterials that can be deployed in a number of fields, including energy, manufacturing and biomedicine.

Krzysztof Matyjaszewski, the J.C. Warner Professor of Natural Sciences and director of Carnegie Mellon's Center for Macromolecular Engineering, was also listed among the most cited researchers in the field of chemistry. Matyjaszewski is known worldwide for developing atom transfer radical polymerization (ATRP), a method that lets scientists carefully structure polymers. With this precision, he and other scientists develop innovative products with a wide range of functionalities.

This year's list includes more than 6,800 individual researchers from universities, research institutes and commercial organizations around the world whose quantitative and qualitative data collected from scholarly publications that ranked in the top 1% of the most cited papers for their subject field.

The evaluation and selection process draws on data from the Web of Science™ citation index, together with analysis performed by bibliometric experts and data scientists at the ISI at Clarivate™.

"The Highly Cited Researchers list identifies and celebrates exceptional individual researchers at Carnegie Mellon University whose significant and broad influence in their fields translates to impact in their research community and innovations that make the world healthier, more sustainable and more secure," said David Pendlebury, head of Research Analysis at the Institute for Scientific Information at Clarivate. "Their contributions resonate far beyond their individual achievements, strengthening the foundation of excellence and innovation in research."

■ *Heidi Opdyke*

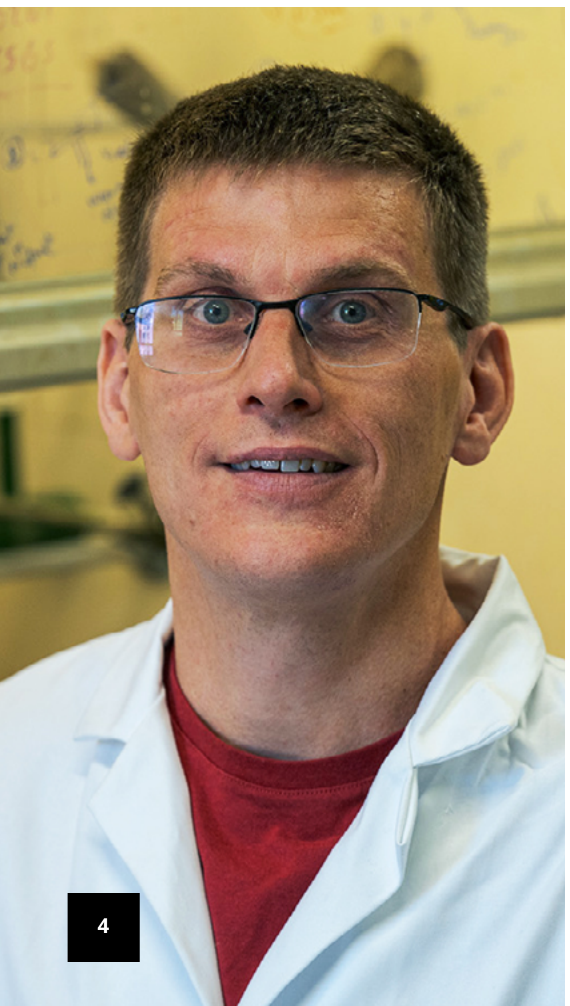
Noonan Named Associate Head of Chemistry

Carnegie Mellon University Professor Kevin Noonan has been named associate head for the Department of Chemistry in the Mellon College of Science. The appointment was effective June 1, 2024.

"Kevin's accomplishments and leadership as a researcher, teacher and mentor made him the ideal candidate for this position," said Bruce Armitage, department head, professor and co-director of the Center for Nucleic Acid Science and Technology.

In his new role, Noonan will oversee the Department of Chemistry's infrastructure and instrumentation and will work with its Graduate and Undergraduate Program Committees on curriculum development.

"I am very excited to help the department move forward with many new, exciting scientific and teaching opportunities in the coming years," Noonan said. "Especially with the new Cloud Lab coming online, the Richard King Mellon Hall of Sciences currently under construction and the chance to develop and integrate new content into our courses."



Noonan has been a faculty member in the Department of Chemistry since 2011. Noonan received his Ph.D. from the University of British Columbia, and prior to joining Carnegie Mellon, he was a postdoctoral fellow at Cornell University. His lab works at the interface of organic, inorganic and organometallic chemistry, and he collaborates with many research groups both at CMU and around the world. He has projects spanning several research areas which are all broadly related to energy research and the environment. Noonan is also a part of the Center for Alkaline-Based Energy Solutions or CABES, a Department of Energy (DOE) Energy Frontier Research Center (EFRC).

In that work, the Noonan lab collaborates with chemists, physicists and engineers to build next generation electrolyzers and fuel cells. In particular, Noonan is developing materials for membranes, a critical component in electrolyzers — devices that use electricity to split water into hydrogen and oxygen. The membrane conducts ions between two electrodes, facilitating the water splitting reaction. The approach is aimed at helping the field move away from precious-metal-based electrocatalysts and dramatically lower the cost of clean hydrogen fuel production by operating in basic media.

A widely respected teacher of numerous core and elective courses for undergraduate and graduate students, Noonan has co-chaired the Department of Chemistry's Graduate Program Committee since 2018. He also provides outreach opportunities for graduate students to work with seventh-12th graders focusing on alternative energy technologies. He is currently a director of the local section of the American Chemical Society (ACS), and he hosts the local ACS Chemistry Olympiad for high school students in the area, a multi-tiered chemistry competition.

■ *Heidi Opdyke*

Sherwood To Lead Undergraduate Studies & Laboratories for Chemistry

Carnegie Mellon University Teaching Professor and Director of Laboratories Gizelle Sherwood has been named director of undergraduate studies for the Department of Chemistry in the Mellon College of Science. The appointment was effective June 1. Sherwood replaces Prof. Karen Stump, who served in that role for 24 years and will retire next summer.

"It's difficult to imagine anyone replacing Karen Stump, who has been the backbone of our undergraduate program for more than two decades, but I'm excited to work with Gizelle in recruiting more majors to our department, broadening our appeal to nonmajors and innovating our curriculum to train students who can tackle the great challenges facing our planet," said Bruce Armitage, Chemistry department head, professor and co-director of the Center for Nucleic Acid Science and Technology.

In her new role, Sherwood will oversee the Department of Chemistry's curriculum and laboratories to ensure that coursework prepares the next generation of scientists. Traditionally, the core role of the director of undergraduate studies is to coordinate and align the undergraduate curriculum with the central missions of the department, the college and the university.

Sherwood (lower left) poses with students in a photo booth at this year's MCS Ball.

"In this role I also hope to be the bridge between the department and our students — chemistry majors as well as anyone who takes a chemistry course," Sherwood said. "As faculty we have a set of expertise. But our students can be empowered to drive their experiences and choices."

Sherwood earned her Ph.D. from Carnegie Mellon in 2008 and joined the faculty as a special lecturer in 2009. In 2014, she was named an assistant teaching professor. She was promoted to associate and full teaching professor in 2019 and 2023, respectively.

Sherwood teaches first and second-year courses such has Modern Chemistry, Laboratory 1: Introduction to Chemical Analysis and Techniques in Quantitative Analysis and helps to build strong foundational knowledge. She also has created and co-taught courses such as The Design and Making of Skin and Hair Products and provides students with real-word applications and opportunities for hands-on learning.

"I am here to be a resource, a tool that students can utilize in their journey on their paths to becoming researchers, doctors, teachers, changemakers... the list can go on and on. In particular, I want to help them understand the place of chemistry in their life's journey. Because it's everywhere!" she said. "Our department is known for being a small tight knit community. I also hope to maintain that level of familiarity and community, established by my predecessors, that has been integral to our departmental success."

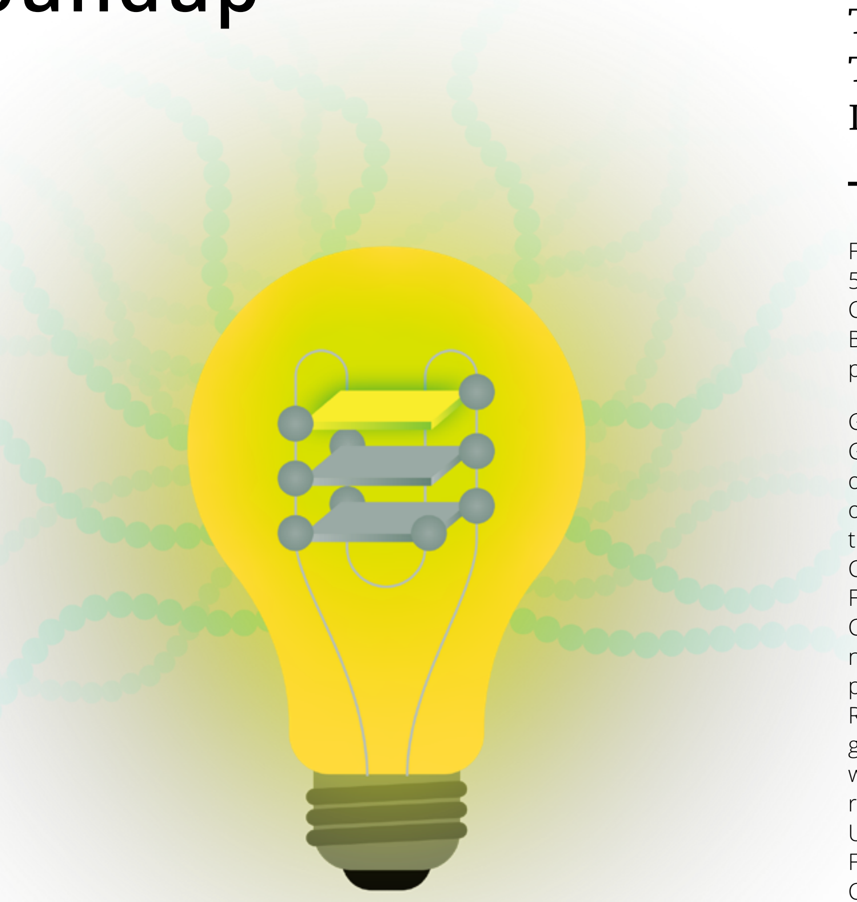
Sherwood is a strong advocate for outreach programs and works with organizations such as Carnegie Mellon's Gelfand Center, Pennsylvania Junior Academy of Science and Boy Scouts of America to develop K-12 outreach programs in chemistry.

Among her accolades, Sherwood was named a Provost's Inclusive Teaching Fellow in 2021 and earned the Julius Ashkin Teaching Award in 2020.

■ *Heidi Opdyke*

Research Roundup

A Bright Idea: Chemists Use Nucleic Acid Binding Dyes as Photocatalysts for ATRP



Researchers in Carnegie Mellon University's Department of Chemistry have developed a nucleic-acid-based photocatalyst that can precisely control atom transfer radical polymerization (ATRP), a popular method used to generate a wide range of materials with highly specific, tailored functionalities. The novel approach took something old — fluorescent dyes that bind to nucleic acids — and turned it into something new — a versatile photocatalyst that allows for precise control over the polymerization reaction.

"Nucleic acid-binding dyes are intriguing fluorescent molecules that illuminate and become activated exclusively in the presence of nucleic acids. Consequently, in our system, polymerization occurs only in the presence of nucleic acids, allowing us to manipulate the process by selecting appropriate nucleic acids as cofactors," said chemistry doctoral student Jaepil Jeong.

The work, published in the Journal of the American Chemical Society, holds promise for advancing the emerging field of nucleic acid-based materials and technologies including logic-controlled photoATRP, nanofabrication and pathogen detection, according to the scientists.

ATRP, the most robust method of controlled polymerization, allows scientists to string together small molecules called monomers in a piece-by-piece fashion, resulting in highly tailored polymers with specific properties. ATRP can be shut down or restarted at will, depending on how the conditions of the reaction are varied.

One way to control the reaction is by using photocatalysts, materials that can change the rate of a chemical reaction by being exposed to light. While there are photopolymerization systems that use simple fluorescent dyes that activate when exposed to light, the Carnegie Mellon team took it one step further using nucleic acid-binding dyes.

This has applications in the fields of nano- and biotechnology for diagnostic and analytical applications.

Jeong is co-advised by Subha R. Das, associate professor of chemistry and a member of Carnegie Mellon's Center for Nucleic Acids Science and Technology, and Krzysztof Matyjaszewski, the J.C. Warner University Professor of Natural Sciences. Along with Jeong, Matyjaszewski and Das, Marco Fantin of the University of Padova is an author on the JACS paper.

■ *Amy Pavlak Laird*

Team Wins Challenge To Advance Parkinson's Disease Research

Familial Parkinson's disease affects at least 500,000 Americans yearly, but a team of Carnegie Mellon University and University of British Columbia researchers have found a potential target for a treatment.

Graduate students Filipp Gusev, Evgeny Gutkin and Ben Koby along with Professor of Chemistry Olexandr Isayev and Professor of Chemistry Maria Kurnikova, were part of the Carnegie Mellon team that took on the Critical Assessment of Computational Hit-Finding Experiments (CACHE) Drug Discovery Challenge #1. The challenge involved using novel computational methods to find potential binding agents for Leucine-Rich Repeat Kinase 2 (LRRK2), the most common genetic cause of Parkinson's Disease. Along with Chamali Narangoda, a postdoctoral researcher in the Kurnikova group, and University of British Columbia collaborators Francesco Gentile, Fuqiang Ban and Artem Cherkasov, the team tied for first place in the challenge.

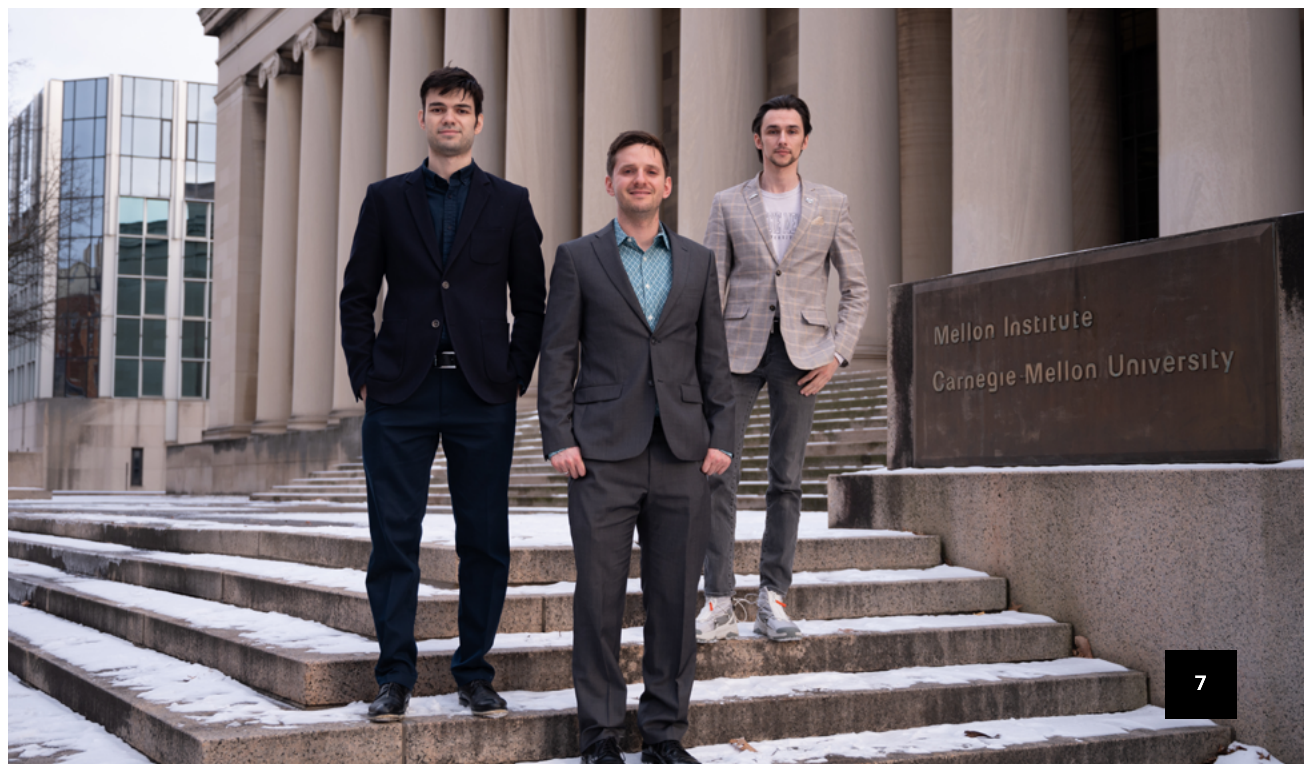
Starting with a database of some 4.5 billion commercially available small molecules and ligands that was narrowed down to 800 molecules by collaborators at the University of British Columbia, the Carnegie Mellon chemists used absolute binding free energy simulations to determine which of the potential molecules would be optimal for experimental validation. The team spent six weeks simulating the candidates with Bridges-2 resources of the Pittsburgh Supercomputing Center.

From the five top molecules, they took two of the most promising candidates and used a machine learning database to select potential analogs and orientations that would be most likely to strongly bind to LRRK2. After each analog was selected, they performed lead optimization, where they again simulated then thoroughly analyzed the candidate to determine its effectiveness.

After submitting the best analogs to the CACHE organizers, they discovered that multiple candidates can inhibit LRRK2. With knowledge about these inhibitors, drug development researchers can use them as a basis for potential Parkinson's disease treatments.

The work received funding from the National Institutes of Health and the National Science Foundation.

■ *Kirsten Heuring*



CMU-Designed Artificially Intelligent Coscientist Automates Scientific Discovery

A non-organic intelligent system has for the first time designed, planned and executed a chemistry experiment, Carnegie Mellon University researchers report in the Dec. 21 issue of the journal Nature (doi:10.1038/s41586-023-06792-0).

“We anticipate that intelligent agent systems for autonomous scientific experimentation will bring tremendous discoveries, unforeseen therapies and new materials. While we cannot predict what those discoveries will be, we hope to see a new way of conducting research given by the synergetic partnership between humans and machines,” the Carnegie Mellon research team wrote in their paper.

The system, called Coscientist, was designed by Assistant Professor of Chemistry and Chemical Engineering Gabe Gomes and chemical engineering doctoral students Daniil Boiko and Robert MacKnight. It uses large language models (LLMs), including OpenAI’s GPT-4 and Anthropic’s Claude, to execute the full range of the experimental process with a simple, plain language prompt.

For example, a scientist could ask Coscientist to find a compound with given properties. The system scours the internet, documentation data and other available sources, synthesizes the information and selects a course of experimentation that uses robotic application programming interfaces (APIs). The experimental plan is then sent to and completed by automated instruments. In all, a human working with the system can design and run an experiment much more quickly, accurately and efficiently than a human alone.

“Beyond the chemical synthesis tasks demonstrated by their system, Gomes and his team have successfully synthesized a sort of hyper-efficient lab partner,” says National Science Foundation (NSF) Chemistry Division Director David Berkowitz. “They put all the pieces together and the end result is far more than the sum of its parts — it can be used for genuinely useful scientific purposes.”

Specifically, in the Nature paper, the research group demonstrated that Coscientist can plan the chemical synthesis of known compounds; search and navigate hardware documentation; use documentation to execute high-level commands in an automated lab called a cloud lab; control liquid handling instruments; complete scientific tasks that require the use of multiple hardware modules and diverse data sources; and solve optimization problems by analyzing previously collected data.

“Using LLMs will help us overcome one of the most significant barriers for using automated labs: the ability to code,” said Gomes. “If a scientist can interact with automated platforms in natural language, we open the field to many more people.”

This includes academic researchers who don’t have access to the advanced scientific research instrumentation typically only found at top-tier universities and institutions. A remote-controlled automated lab, often called a cloud lab or self-driving lab, brings access to these scientists, democratizing science.

The Carnegie Mellon researchers partnered with Ben Kline from Emerald Cloud Lab (ECL), a Carnegie Mellon-alumni founded, remotely operated research facility that handles all aspects of daily lab work, to demonstrate that Coscientist can be used to execute experiments in an automated robotic lab.

“Professor Gomes and his team’s groundbreaking work here has not only demonstrated the value of self-driving experimentation but also pioneered a novel means of sharing the fruits of that work with the broader scientific community using cloud lab technology,” said Brian Frezza, co-founder and co-CEO of ECL.

Carnegie Mellon, in partnership with ECL, opened the first cloud lab at a university in 2024 and will eventually give the university’s researchers and their collaborators access to more than 200 pieces of equipment. Gomes plans to continue to develop the technologies described in the Nature paper to be used with the Carnegie Mellon Cloud Lab, and other self-driving labs, in the future.

Coscientist also, in effect, opens the “black box” of experimentation. The system follows and documents each step of the research, making the work fully traceable and reproducible.

Safety concerns surrounding LLMs, especially in relation to scientific experimentation, are paramount to Gomes. In the paper’s supporting information, Gomes’s team investigated the possibility that the AI could be coerced into making hazardous chemicals or controlled substances.

“I believe the positive things that AI-enabled science can do far outweigh the negatives. But we have a responsibility to acknowledge what could go wrong and provide solutions and fail-safes,” said Gomes.

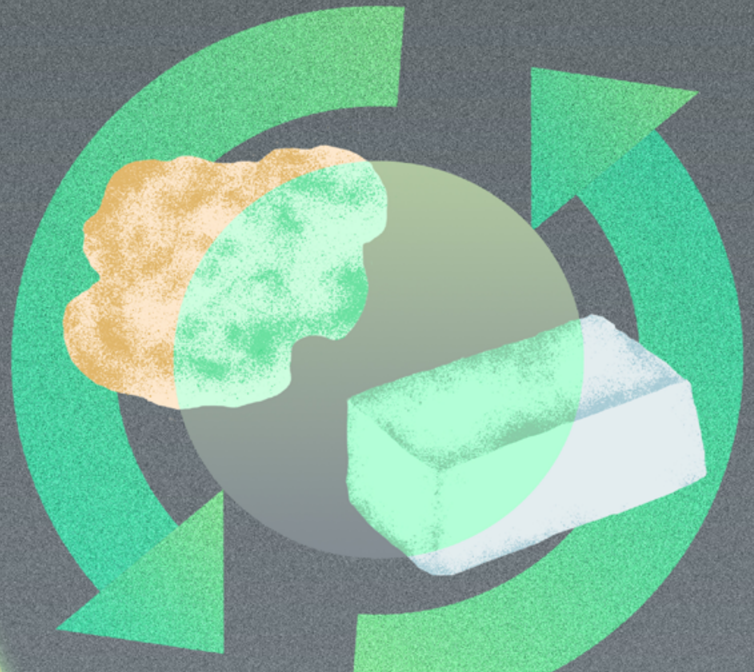
“By ensuring ethical and responsible use of these powerful tools, we can continue to explore the vast potential of large language models in advancing scientific research while mitigating the risks associated with their misuse,” the authors wrote in the paper.

■ *Jocelyn Duffy*

Research Feature

A Greener Future Through Sustainable Catalysis

by Amy Pavlak Laird



Catalysis has had a transformative impact on the chemical industry and society at large. The process has been indispensable in producing everything from fuels to pharmaceuticals. The linchpin to most of these compounds is typically precious-metal catalysts. But these metals come with a high price tag and a high carbon footprint.

As chemists strive for a more sustainable future, they are looking to earth-abundant and especially biochemically common transition metals such as copper and iron as green alternatives. Earth-abundant metals are plentiful, so they are less costly and less carbon intensive to refine, and biochemically common metals tend to be less toxic. And nature already cleverly uses them to do extraordinary chemistry.

"Metals such as iron, copper, manganese, calcium and potassium are critical for natural catalytic process," said Isaac Garcia-Bosch, associate professor of chemistry. "For example, our liver uses iron catalysis to process pharmaceuticals, and trees use manganese catalysis during photosynthesis to transform water into the oxygen that we breathe."

A broad group of enzymes containing metal ions are known as metalloenzymes, which play a vital role in many essential metabolic processes. They enable efficient and reversible reactions under mild conditions — a goal synthetic chemists strive to meet. But recreating the powerful functions of metalloenzymes in the lab is a daunting task, said Garcia-Bosch. Due to their structural complexity, the specific active sites, reaction mechanisms and intermediates of many of these enzymes, especially copper ones, are still not well known. This is where synthetic inorganic chemists like Garcia-Bosch can help by synthesizing model copper compounds as analogues of the enzymes' active sites.

"Model systems are very, very helpful in terms of determining the structure and the kind of intermediates that are formed for some of these metalloenzymes," Garcia-Bosch said. "But we're also trying to take the next step, which is: can we use these copper compounds to do useful synthetic organic chemistry."

Garcia-Bosch's lab is developing copper (Cu) complexes that can do selective carbon-hydrogen (C-H) hydroxylation reactions. C-H bonds are quite strong, so doing a selective hydroxylation and putting an oxygen on a specific C bond opens up an organic chemists' options for making a wide variety of useful compounds. He said building metal complexes that can oxidize selectively at a particular position is very challenging, especially since his lab is using hydrogen peroxide (H_2O_2) as the oxidant. Because solutions of H_2O_2 are stable, it is more practical to use, plus it's a stronger oxidant than oxygen. One of the main challenges of this approach is that H_2O_2's reactivity with metals can lead to the formation of Fenton oxidants, which can oxidize most bonds, leading to non-selective oxidations. Nature, including metalloenzymes like lytic polysaccharide monooxygenases, has evolved to bypass these issues.

"To control the reactivity, our lab uses directing groups to select what C-H bond we want to oxidize," he said. "Our work has been focusing a lot on this approach because it is becoming more apparent that that's what metalloenzymes do — a substrate coordinates to the active site of the metalloenzyme before the oxidant is introduced."

In research published over the last few years, Garcia-Bosch and collaborators developed a synthetic protocol for the functionalization of ketones (and aldehydes) using directing groups, copper and H_2O_2. The reaction resulted in remarkable C-H hydroxylation yields with unprecedented selectivities. While the lab used the directing group approach to do sp^3 hydroxylations, the team recently published several papers doing sp^2 C-H hydroxylation reactions. They also have shown that they can change the identity of the hydroxylation product by changing the directing group that's used.

Garcia-Bosch said that doing selective hydroxylations using copper and hydrogen peroxide seemed impossible just a few years ago. Now it's not only possible but his lab has developed a simple protocol to make it happen easily and inexpensively. Typically in copper chemistry, chemists need to work in an environment — like a glovebox — free of water and oxygen, but with Garcia-Bosch's protocol using directing groups, the Cu(I) and Cu(II) precursors used are stable in air, so a glovebox isn't necessary.

And now, people from outside the field are using Garcia-Bosch's protocols to do these types of Cu (II)-mediated organic syntheses.

"People are using our protocols to do selective hydroxylations to synthesize complex molecules, and that makes me very proud," he said.

Garcia-Bosch also is looking to copper-containing enzymes for new ways to promote useful oxidations of hydrocarbons. He's particularly inspired by particulate methane monooxygenase (pMMO), a membrane-bound enzyme that catalyzes the oxidation of methane to methanol in methanotropic bacteria.

"It's a really cool transformation because this metalloenzyme can transform methane to methanol at room temperature using oxygen. This is probably one of the most challenging organic transformations and it has a lot of application in industry. We would like to take the methane that comes from extracting oil, for example, and take it to methanol, a liquid that we can use for organic synthesis."

To mimic nature's catalysis, Garcia-Bosch is developing copper complexes as oxidation catalysts to tackle some of these challenging transformations, such as the functionalization of C-H and C=C bonds, under mild conditions using cheap and non-toxic reagents. Like some of their natural counterparts, the catalysts contain a redox-active ligand with tunable H-bonding donors, which allows for control of the reactivity of the intermediate species that are formed during these transformations. The long-range goal is to discover new synthetic routes to compounds that could be useful as pharmaceuticals, polymers and other industrially useful chemical compounds.

Collins and Ryan Sullivan, professor of chemistry and mechanical engineering, co-founded Sudoc, a startup focused on developing and commercializing TAML catalysts for use in everything from cleaning products to solutions for wastewater treatment and remediation. In a process that is so simple that it can be used almost anywhere, TAML catalysts remove from water sources myriad persistent pollutants that often escape water treatment, including endocrine-disrupting pharmaceuticals and pesticides, fossil carbon industry residuals and antiozonant tire wear particles that are deadly to coho salmon.

STRENGTH IN SUSTAINABILITY

Garcia-Bosch's arrival at Carnegie Mellon two years ago adds to the Department of Chemistry's faculty strengths in the fields of metalloproteins and green chemistry, including two Presidential Green Chemistry Challenge Award winners who have for years been looking to nature for inspiration in the lab.

Terry Collins, the Teresa Heinz Professor of Green Chemistry and director of the Institute for Green Science at Carnegie Mellon, has dedicated his career to developing methods to remove synthetic chemicals from water. Inspired by the way peroxidase enzymes work in the human liver to destroy hazardous compounds, Collins invented TAML® (tetraamido-macrocyclic ligand) catalysts.

"We had to make the iron center of our catalysts do the same kind of chemistry as the iron center of the peroxidase enzymes," said Collins, who successfully did so and has continued to develop TAMLs for environmentally sustainable and efficient use over the last three decades.

TAMLs catalytically activate hydrogen peroxide to eliminate micro-pollutants and pathogens from water. By mimicking oxidative metabolism, TAMLs' oxidation processes can be used for cleaning, water treatment and the removal of recalcitrant toxic chemicals like endocrine disrupting chemicals, active pharmaceutical ingredients, pesticides and more. These discoveries are underpinning new technologies for treating diverse wastewaters and enabling other products, such as cleaning products for mold remediation.

The U.S. Environmental Protection Agency (EPA) recognized Collins' work with the Presidential Green Chemistry Challenge Award in 1999. Ten years later, the EPA again honored a Carnegie Mellon chemist with the award. Krzysztof Matyjaszewski, J.C. Warner University Professor of Natural Sciences, was recognized for his development of an environmentally low-impact form of atom transfer radical polymerization (ATRP) — a widely used method for the preparation of functional polymers.

In 2023, the National Academy of Sciences named Krzysztof Matyjaszewski the recipient of the NAS Award in Chemical Sciences for his trailblazing and transformative advancements in polymer chemistry.

ATRP, which was developed by Matyjaszewski, relies on a specialized copper catalyst to synthesize well-defined polymers with precisely controlled molecular architectures. The process is used in industry to create polymers that are employed as components of everything from coatings and surfactants to applications in medicine and electronics. The success of ATRP in creating such a range of commercial products has motivated Matyjaszewski to develop more efficient, environmentally friendly and scalable ways that minimize ATRP's environmental impact.

In the early stages of ATRP development, high levels of copper catalyst were required to maintain the process. To lessen the amount of copper catalyst needed, Matyjaszewski's group introduced an approach that incorporates environmentally benign reducing agents, like vitamin C and sugars, to regenerate the active form of the catalyst. They've also used external stimuli, including electrical currents, light, mechanical forces and ultrasound, to regenerate the copper catalyst. These techniques, which reduce the level of copper to a few parts per million, have allowed not only for less catalyst to be used, but also for increasing the oxygen tolerance of the polymerization and developing systems to conduct ATRP in open air. Together, these advances offer a promising approach for creating specialized polymers in greener and more practical ways.

Catalysts will play a pivotal role in achieving a greener future. Carnegie Mellon chemists are tackling some of the grandest challenges in catalysis science through bio-inspired design and cost-saving, greener reaction pathways. Together these advancements are promising steps toward more sustainable catalysis for a better tomorrow.

Student Stories

Chemists Test Museum Artifact To Identify Resin Ingredients

To learn about something old, curators at Carnegie Museum of Natural History turned to something new at Carnegie Mellon University.

"Studying the past is complicated and requires the work of all kinds of experts. I love collaborating with other people," said Lisa Saladino Haney, Egyptologist and assistant curator at Carnegie Museum of Natural History.

Carnegie Museum of Natural History has more than 22 million objects in its care. Of those, the museum stewards approximately 5,000 objects and 17 individuals from the Nile Valley. Haney said most of the material comes from Egypt, including the cup.

Burning incense was a daily occurrence in ancient Egypt used in rituals, healing and daily life. Among the substances used were frankincense and myrrh as well as mixtures that included herbs, spices and gums made from tree resin.

The cup was likely used in temple ceremonies, possibly as a storage container since the residue was still white and does not appear to have been burned, Haney said.

"Residue analysis is something that requires special expertise and equipment, so it isn't always possible to do," Haney said. "There are many different types of residue analysis. Often it can help you see how something was made, what it may have been made of — or in the case of a cup, what it may have originally contained — or how it was used."

Travis Olds, assistant curator of minerals in the Section of Minerals and Earth Sciences at CMNH, reached out to Mark Bier, a research professor in chemistry and director for the Center Molecular for Analysis at Carnegie Mellon, to see if he could help study the cup.

Bier responded. With more than a dozen patents related to mass spectrometry, Bier and his lab are working to build improved instrumentation and methods to determine the mass of different molecules in a sample.

Nicole Auvil is a doctoral researcher in the Department of Chemistry and a member of Bier's group. She and Bier used a "super-sniffer" they developed to test a sample of residue from a 2,500-year-old bronze cup used to hold incense.

In Auvil's first semester, she figured out how to reproducibly make ultrasharp needles out of tungsten metal and further developed a mass spectrometer ionization source with which to use them.

"That was a tricky task," she said. "At the time, we didn't know if it would be possible to make needles this sharp... and to make them reproducible? I knew I was taking on a project that might not be successful."

The needle's job is to emit a highly energetic plasma called a corona discharge. The sharper the needle, the lower the voltage it requires do to this job. Corona discharge ionizes the ambient air (and whatever molecules it may contain) in a small region around the needle tip — a proton is added or one or more electrons are knocked off to create positive ions.

The ions are then sucked into a vacuum chamber and into a mass analyzer for mass-to-charge analysis and detection. For a linear ion trap mass analyzer — one of Bier's most impactful inventions — this is accomplished by measuring the point of radial ion ejection of each ion out of the trapping region. The instrument records the relative abundances of an ion's mass-to-charge ratio to produce a visual read-out called a mass spectrum.

Commercial needles used for atmospheric pressure chemical ionization typically have a tip radius greater than 14 microns at their sharpest point. Through an electrochemical etching process adapted from methods found in the literature, Auvil made her needles extremely sharp — just 18 nm at their point. She and Bier have filed a provisional patent on the device. With the needle question resolved, the "super-sniffer" was put to work on many sample types.

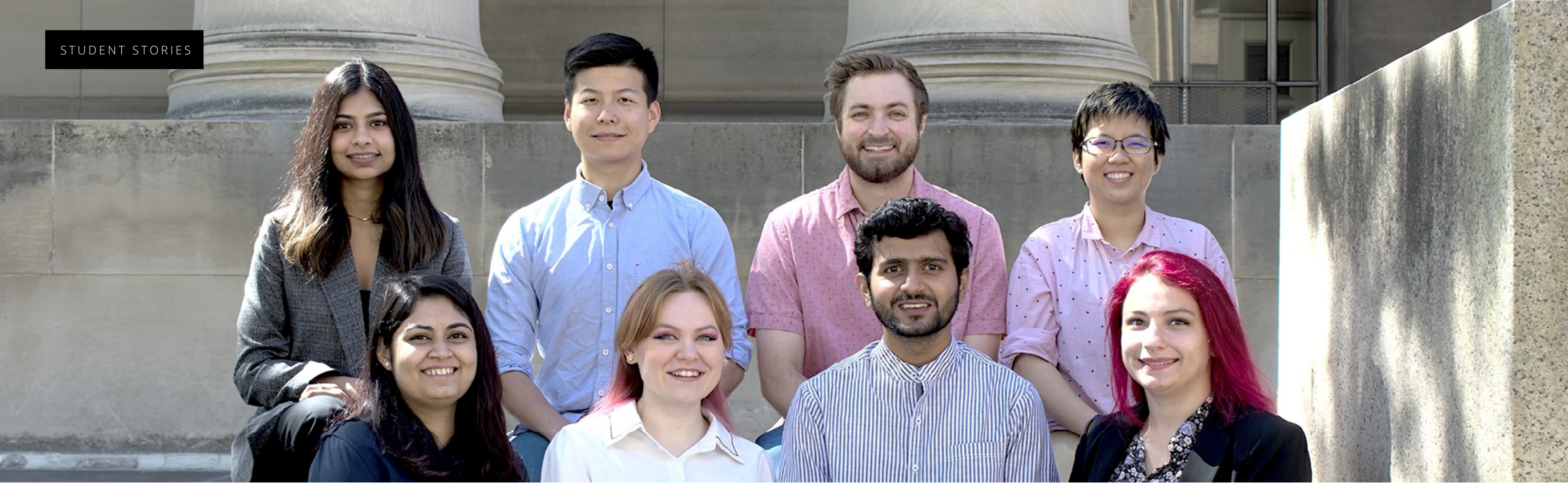
"Twenty minutes after drinking a cup of coffee, the sniffer can detect caffeine coming out of your pores," Auvil said. "My graduate career will include further development of this ionization source as well as adapting it for specific applications such as imaging, air quality monitoring, breath analysis and nicotine vape analysis."

Before testing on the cup could begin, Bier and Auvil walked the cup between the museum and Bier's lab. It was the first time the cup left the museum in 30 years.

"Taking into account the molecular weight, isotopic distribution, the software-suggested molecular formulae and the literature, we were able to tentatively identify this molecule as Arabinonic acid," Auvil said. Also known as Arabic acid, the molecule can be found as a degradation product of the simple sugar arabinose, which can be found in Arabic gum from acacia trees and in cannabis sativa, both native to Egypt.

"Although exciting, we need to do more experiments to gain confidence in this identification," Bier said. "It was just such a unique and valuable sample and the people at the museum were equally excited about the possibilities of our work."

■ *Heidi Opdyke*



Chemistry Ph.D. Students Host ACS Symposium

Carnegie Mellon University doctoral student Savannah Talledo directed plays at Wofford College where she studied theater and chemistry as an undergraduate. In August 2023, Talledo took on a new form of direction — producing a symposium at the American Chemical Society (ACS) Fall 2023 Meeting.

“With theater, you direct plays, and the symposium was kind of like that,” said Talledo, a member of the Bernhard group in the Department of Chemistry. “It was challenging but exciting to be in charge of something like this and have this responsibility. It was a great leadership experience.”

Talledo spearheaded the graduate student committee that organized Catalyzing Collaboration: Bridging the Gap between Machine Learning, Computational Modeling and Experimental Chemistry for Catalyst Design. The committee’s goal was to create a daylong event that brought together chemists who share the goal of studying transition metal catalysis. They said they hoped their symposium would encourage attendees to collaborate more across universities and disciplines and to consider new research tools.

“We’re all doing catalysis, and we want to bridge the gap between machine learning, computational modeling and experimental chemistry,” Talledo said.

Talledo first heard about the opportunity during her first year of her Ph.D. program. ACS has a Graduate Student Symposium Planning Committee (GSSPC) create a daylong symposium as part of its annual fall conference. Talledo saw it as an excellent chance to learn what goes into creating a symposium. She brought together Ph.D. students from multiple labs to write a proposal in spring 2022 including Xiaolei Hu, a member of the Matyjaszewski group, and Jess Vinskus, a member of the Noonan group. After their proposal was accepted, they got to work.

The students suggested potential speakers and oversaw the whole symposium. So the team could ensure speakers and students could attend, Hu advertised and fundraised for the symposium.

“Starting from proposing the symposium to organizing the whole day’s schedule for the conference was a totally new experience with me,” Hu said. “I worked with an amazing team, and I learned a lot from the whole experience.”

Vinskus sent letters to sponsors, managed their symposium Instagram account and created graphics and a banner.

“We put in all this work, we did all this research and we planned everything. Watching it all come together, watching the speakers give their talks, it was so rewarding,” Vinskus said.

On the day of the symposium, there was a series of eight researchers from around the United States, including Dr. Malika Jeffries-El., professor of chemistry and associate dean of the graduate school of arts and sciences at Boston University and a former postdoctoral researcher at Carnegie Mellon. Jeffries-El presented a talk entitled Design and Synthesis of Organic Electronic Materials.

“She was a researcher who I was interested in and that I brought to the table,” Vinskus said. “She was a really great speaker. I found the synthetic chemistry she was working on really interesting because it’s similar to what she did on conjugated polymers in her postdoc at CMU.”

Another speaker was David Cabanero, a Ph.D. student in chemistry at Columbia University working with Tomislav Rovis. When Rovis was unable to come to the conference, Cabanero stepped in, giving a talk entitled Collaboration in Academia — New Tools for Catalysis.

“He did an excellent job presenting the research he and his group did,” Hu said. “His presentation was relevant to my research topic as well, and I learned a lot from it.”

Along with organizing the symposium, many of the students involved in the committee, including Talledo and Vinskus, presented at the ACS Fall Meeting. Talledo gave a poster presentation, and Vinskus gave a twenty minute talk.

“I gave a talk on my sulfur compounds, which are called sulfoxoniums and sulfoximines,” Vinskus said. “I’m working on functionalizing them onto polymers and monomers. I think the talk went really well, and I had some good questions on my work.”

After the ACS Fall Meeting concluded, Talledo said that she was proud of what the committee achieved, and she was thankful for the team she worked with.

“The process was fun, and we had a great team,” Talledo said. “I’m glad I had that experience.”

■ *Kirsten Heuring*

Colin Martin Competes in U.S. Olympic Marathon Trials

Chemistry doctoral student Colin Martin spent the cold, dreary days of a Pittsburgh winter powering through 14 runs a week as he trained for the U.S. Olympic Marathon Trials, held on Feb. 3, in Orlando, Florida.

In June 2023, Martin ran the Grandma's Marathon in Duluth, Minnesota, with a time of 2 hours, 17 minutes and 28 seconds, which met the qualifying threshold for the U.S. Olympic trials.

"This is the biggest goal I've ever set for myself and to achieve it was really special," Martin said.

Martin was one of hundreds of runners hoping to represent the U.S. at the 2024 Summer Olympics in Paris. Leading up to the big race, he worked on managing expectations.

"Everyone comes up to me and they go Colin, you're going to the Olympics, you're going to the Olympics! And I always have to slow them down and be like probably. And by probably, I mean definitely not," he joked. "It's a very, very long shot."

Only the top three men and top three women make the United States team.

"For me to be able to reach that level, I would need to quit school and do nothing but run all the time, every day," Martin said. "And I love science, so I'd rather do both and just enjoy."

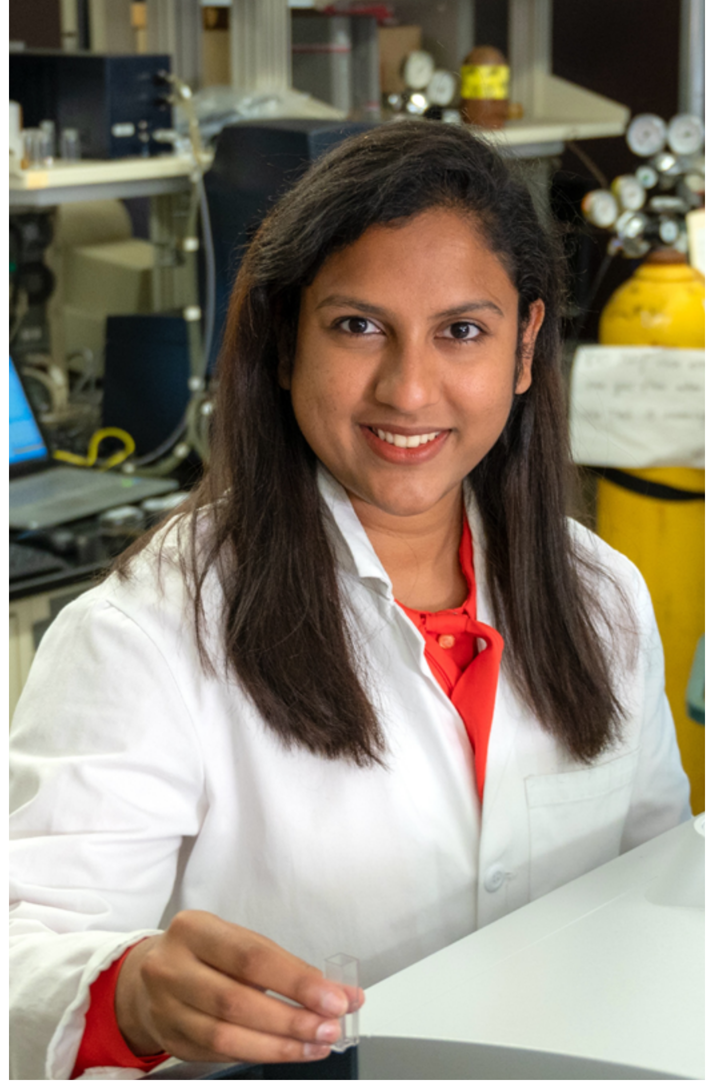
Martin, who is a fourth-year Ph.D. student in Chemistry Professor Bruce Armitage's lab, conducts research related to peptide nucleic acid synthesis and its applications to human disease therapies.

Martin, whose goal was to finish among the top 100, finished 68th. He was thrilled to run in the Orlando race, one of the most competitive distance-running races in the country, with his family, his fiancée Sarah and his friends cheering him on.

"They're incredible people to have around," he said. "I wouldn't have been able to do this without them."

■ *Amy Pavlak Laird*

Colin Martin (far right) competes in the Grandma's Marathon in Duluth, Minnesota.



Kriti Kapil Receives Kwolek Fellowship

Kriti Kapil believes that polymers can be for everyone, and her research is helping to make that possible.

"The most exciting thing is that the technique is incredibly user-friendly. Anyone, regardless of their background as a chemist, can use it," said Kapil, a recent Ph.D. graduate from Carnegie Mellon University's Department of Chemistry. "It opens the door for researchers from interdisciplinary fields to delve into the realm of polymers, allowing them to expand the scope of their research by varying polymer compositions, architectures, and functionalities for diverse applications."

Polymers are a large group of natural and synthetic substances composed of repeating patterns of smaller, monomeric molecules. Synthetic polymers have a variety of applications from nylon and polyester, which are used to make products such as clothes, car tires and glue.

Kapil works to develop oxygen-tolerant polymerization systems, which would allow polymers to be created in less stringent conditions with less complex equipment. This would allow the atom transfer radical polymerization (ATRP) technique designed by Krzysztof Matyjaszewski, J.C. Warner University Professor of Natural Sciences, to be activated by visible light in aqueous environments.

"This work took away all the complexities of the setup and equipment that was necessary in the beginning," Kapil said. "Photo-ATRP is a rapid, practical and simple technique that enables well-controlled polymers for broader use."

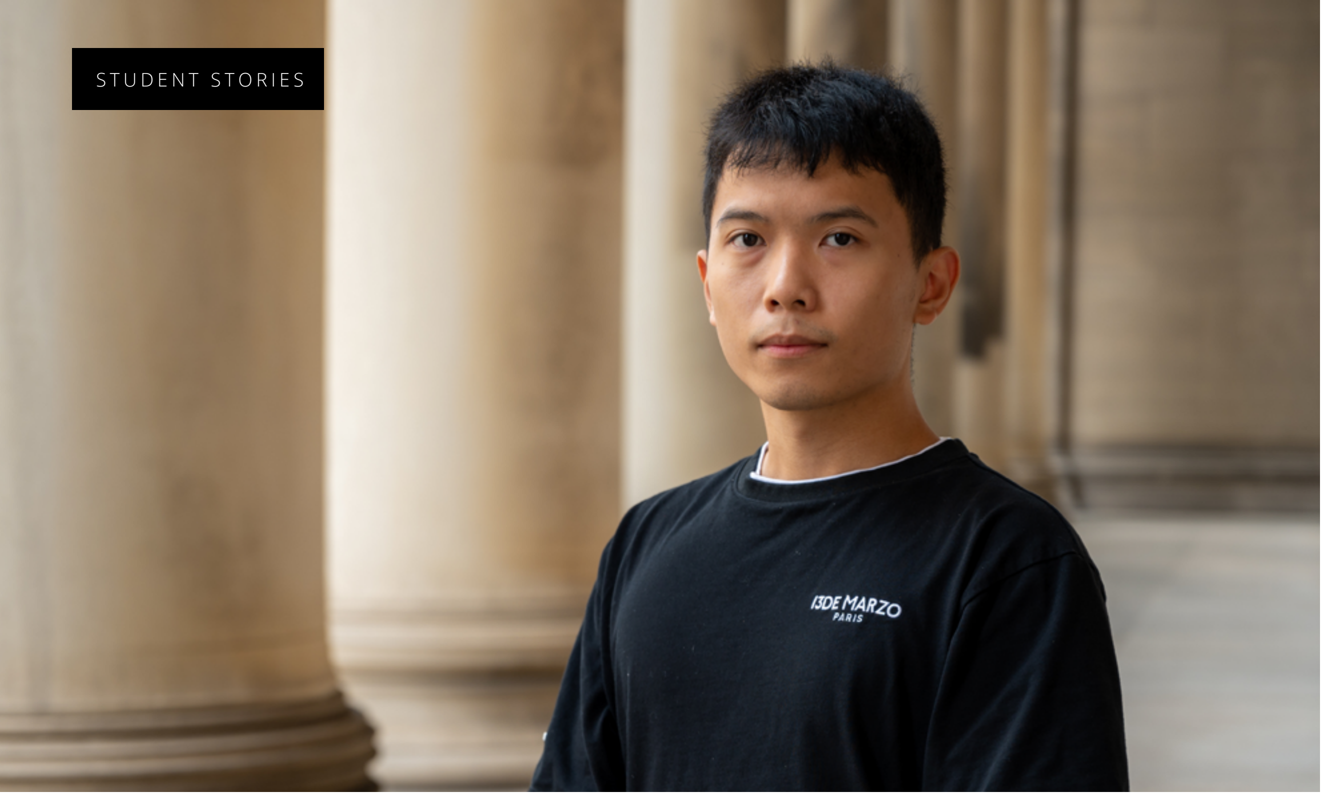
Kapil has shared her research with a wider audience from academia and industry through presentations at the Gordon conference, the ACS National Meeting and during Controlled Radical Polymerization consortium meetings. Her work was recognized both in and outside the Matyjaszewski Group, leading to multiple publications.

Because of her work, Kapil received the Kwolek Fellowship in Chemistry. The fellowship is awarded to women working toward their Ph.D. in chemistry who have demonstrated significant advances in their research. She said she hopes to use her career to further advance polymer development.

"One day, I think all of these methods will be adopted by industries, and that would make polymer creation a lot greener, less time-consuming, less expensive, and much safer because it requires fewer chemicals," Kapil said. "I'm excited to see that all come into action one day."

Kriti successfully defended her thesis in May and is now working at Dow Chemicals in Midland, MI.

■ *Kirsten Heuring*



Zhongyu Liu Receives IPMI Student Award

Chemistry Ph.D. student Zhongyu Liu received the 2024 Bureau Veritas Student Award from the International Precious Metals Institute (IPMI) for his work on the photoluminescence of ultrasmall gold nanoclusters. He received the $5,000 award at the IPMI's annual conference.

Liu's research focuses on atomically precise gold nanoclusters made of only dozens of atoms. These nanosized particles have unique optical, electrical and magnetic properties. Of particular interest to Liu is their photoluminescence.

"Gold nanoclusters are very special materials with intriguing optical properties," Liu said. "What interests me is understanding their unique emission range and how to manipulate their emission intensity."

By manipulating the nanoclusters' size, structure and composition, they can be tuned to emit wavelengths from the visible to the near-infrared regions of the electromagnetic spectrum. Developing molecules that emit in the near-infrared offers advantages in a variety of biomedical imaging applications. Unlike visible light, near-infrared wavelengths can penetrate tissues more deeply owing to much less absorption by biological tissue and dramatically improve the image resolution by minimizing the biological tissue's autofluorescence and optical scattering backgrounds.

Since joining Chemistry Professor Rongchao Jin's group in 2019, Liu has worked to understand the mechanism behind the near-infrared photoluminescence of gold nanoclusters, including $Au_{25}(SR)_{18}$ — a nanocluster with 25 gold atoms surrounded by a ligand shell. He developed a physical model to explain how nanocluster vibrations quenched the luminescence. From there, he designed a strategy to significantly boost the photoluminescence quantum yield, which was a thrilling discovery, according to Jin.

"Zhongyu's work on the photoluminescence of atomically precise gold nanoclusters is highly impactful in both fundamental research and practical applications for bio-imaging," Jin said. "He has carried out exceptional physical chemistry research, and I'm sure he will make more discoveries."

■ *Amy Pavlak Laird*

Leenia Mukhopadhyay Awarded Steinbrenner Fellowship

Leenia Mukhopadhyay wants to make a lasting impact on per-and polyfluoroalkyl substances (PFAS) research.

"PFAS, which are also known as 'forever chemicals,' are widespread in nature and basically everywhere," said Mukhopadhyay, a graduate student in Assistant Professor Carrie McDonough's lab in the Chemistry Department. "They are very slippery and long-lasting. They're mostly present in nonstick pans, food packaging, microwave popcorn and anything that's waterproof."

Despite being useful as a nonstick coating, PFAS are toxic to humans and wildlife. In humans, PFAS can cause developmental delays in children, increase the risk of some cancers and reduce the immune system's effectiveness.

Because these molecules are designed to be sturdy, they can persist for years in the environment and in organisms, with higher levels of PFAS being more dangerous for nearby organisms. But, Mukhopadhyay said researchers cannot effectively measure the levels of PFAS in waterways while conducting fieldwork, so they cannot see how nearby waterways and marine organisms have been contaminated.

Any affected marine organisms could have broader impacts for organisms up the food chain. For example, clams harvested from an area with high levels of PFAS could be eaten by humans, who may become sick.

Mukhopadhyay wants to create a test to allow people to sample sediment by a body of water and measure the levels of PFAS. This would allow anyone, from researchers to fishermen, to determine if a waterway is safe.

Because of Mukhopadhyay's work, she was awarded a Steinbrenner Doctoral Fellowship through Carnegie Mellon's Steinbrenner Institute for Environmental Education and Research, which aims to change the way the world thinks and acts about the environment. These fellowships are awarded to second year Ph.D. students who are involved in environmentally focused, interdisciplinary research projects.

Mukhopadhyay plans to use the funding to further dive into her research. She said she hopes her work can help both humans and the environment.

"We all want to do our part for the environment. Research is doing my small part," Mukhopadhyay said.

■ *Kirsten Heuring*

Rafael Guzman-Soriano Wins K&L Gates Prize

The future is bright for Rafael Guzman-Soriano, Carnegie Mellon University's 2024 K&L Gates Scholar, whose time at Carnegie Mellon left him feeling prepared for what's next.

The $5,000 prize is given to one graduating undergraduate student who has inspired their fellow students to love learning through a combination of intellect, scholarly achievement, engagement with others and character.

Guzman-Soriano, a recent chemistry graduate, started college in the fall of 2020, at the height of the COVID-19 pandemic when students took courses remotely because of social-distancing guidelines.

In addition to loneliness, he said he experienced imposter syndrome despite earning top marks in his courses. Support from Carnegie Mellon faculty helped him through.

His academic adviser, Karen Stump, recommended him for the Mellon College of Science's Leadership Development Seminar, taught by Michael Murphy, distinguished service professor and executive director of the Center for Leadership Studies. The seminar empowered him.

"One takeaway from the seminar was a lesson on phrasing your success," he said. "I used to say 'I got lucky' a lot, but it's more, like, 'being ready.' I use the skills, resources and everything that I've learned from prior experiences to seize opportunities and succeed in them."

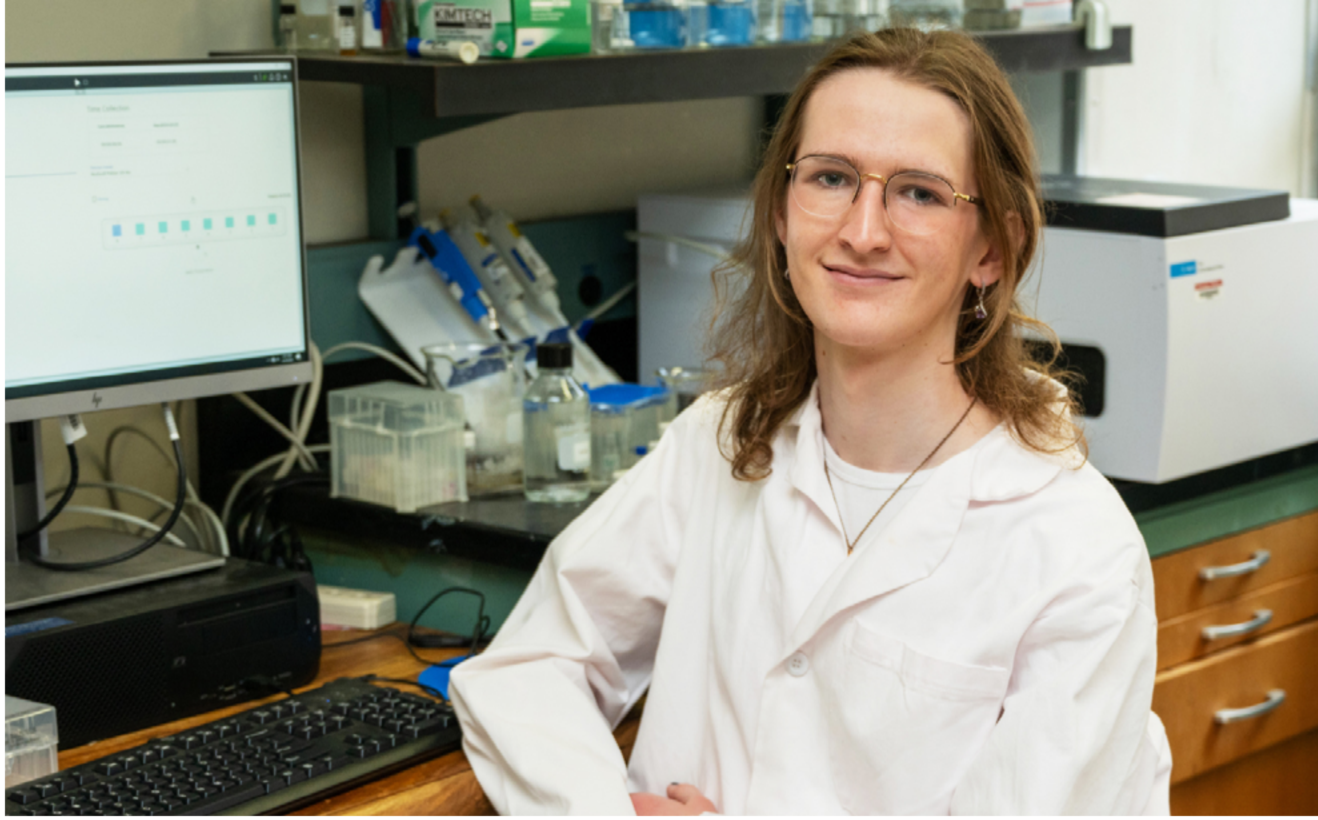
When he became a Tartan Scholars Ambassador and a peer tutor in the Student Academic Success Center in 2022, Guzman-Soriano said he was determined to help other students avoid the struggles he experienced.

"After some time and practice, I gained the trust of these students, and they were trusting of my ability to teach them," he said.

Guzman-Soriano discovered his own happy place in the chemistry lab. During his first year, he took a junior-level course in inorganic chemistry and was invited to work in Chemistry Professor Stefan Bernhard's lab group. His work earned a 2021 NASA Pennsylvania Space Grant Consortium Undergraduate Scholarship.

Guzman-Soriano worked with Bernhard to develop an oxygen sensor. He presented his work to the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers and the American Chemical Society.

■ *Ann Lyon Ritchie*



Minerva Schafer Aims for a Sustainable Life

Recent Carnegie Mellon University graduate Minerva Schafer knows that chemistry done without sustainability in mind can be massively harmful to humans and the environment. Similarly, achievements without self-care may not be sustainable.

When she came to Carnegie Mellon, her plan was to attend graduate school right away.

"Around the time of the application cycle, I decided to take a gap year and focus on self-care," said Schafer, who graduated in May with a major in chemistry and a secondary major in environmental and sustainability studies.

Schafer came out as transgender in the fall of 2023. Her peers selected her to speak at the Department of Chemistry diploma ceremony, and she spoke about her experience.

"Coming out in my senior year was kind of the hardest decision I ever made," she said. "But I made the decision, and my life is so much better for it in so many ways."

She said for anyone facing a difficult decision, sometimes it's not about the facts.

"Sometimes you just need to trust your emotions as a guide and look to people in your life you can trust to navigate the changes with you," she said.

She found a community in Pittsburgh and Carnegie Mellon that has helped support her as she moves forward. For the next year she will continue her research at the Institute for Green Science and the Collins Lab while applying to Ph.D. programs.

Directed by Terrence J. Collins, the Teresa Heinz Professor in Green Chemistry, the lab designs catalysts known as TAMLs that break down various micropollutants and have environmental applications. Schafer has been evaluating the use of TAMLs, environmentally friendly catalysts, for applications in wastewater treatment.

"It's easier to think about how I feel prepared for going forward now," she said. "I still very much like chemistry and chemistry research, but some of the other things I've explored through environmental and sustainability studies tie together interests such as environmental history, policy and rhetoric."

■ *Heidi Opdyke*

Payton Downey Wins Niccolai-Fustanio and Fugassi and Monteverde Awards

Payton Downey lights up when it comes to chemistry research.

"I'm doing work on compounds and their photochemical properties," said Downey, a recent graduate in chemistry with a minor in physics. "I like understanding things, so this is nice to look at things no one else has thought of."

Downey worked with Stefan Bernhard, professor of chemistry, to investigate how and why certain chemicals absorb and refract light.

Light can be polarized to rotate to the left or the right. In an ordinary light fixture, such as a lamp, the rotation cancels out. However, certain chemicals known as chiral luminophores can polarize the light depending on the orientation of their functional groups. The same molecule can affect light in different ways depending on its chiral form.

Downey developed machine learning techniques to investigate why this is the case. In the course of their research, they used computational models to find that the chiral molecules constantly spin around their bonds, which affects luminescence.

Outside of the lab, Downey was most involved in the Carnegie Mellon chapter of PRISM, an LGBTQ+ student organization with chapters across the country. They first joined the group their first year of college.

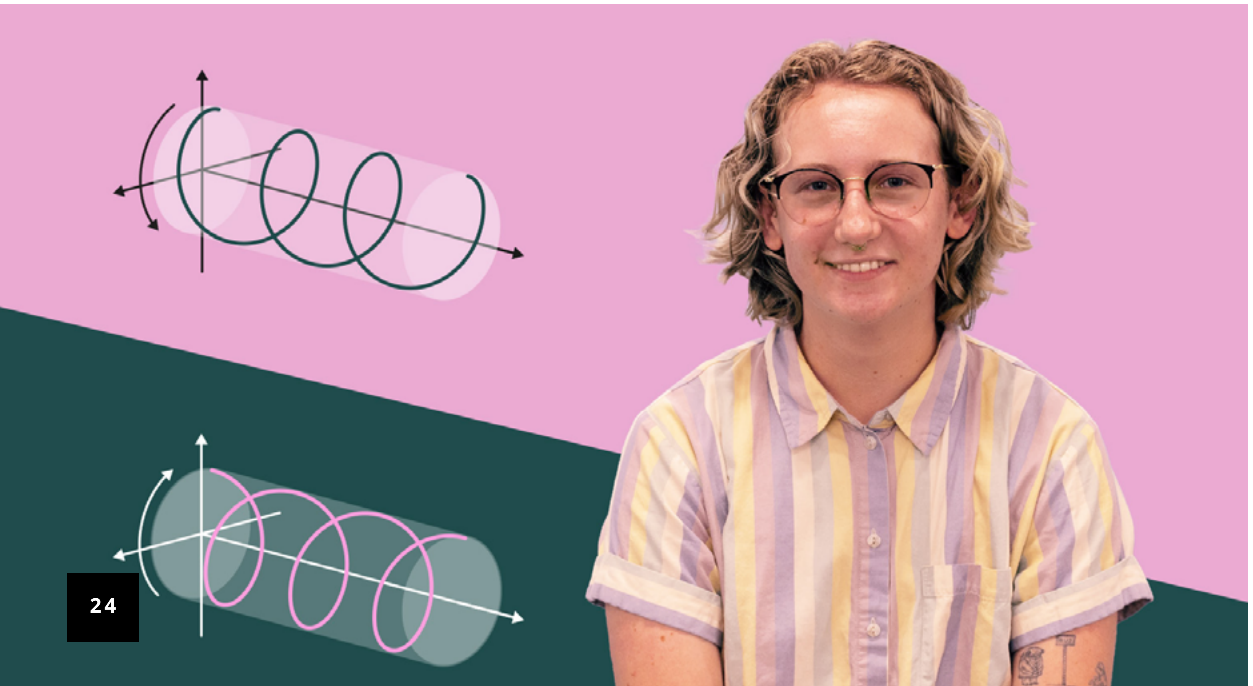
During the COVID-19 pandemic, Downey said that PRISM allowed them to connect with their fellow students at a time where it was difficult to find friends and community elsewhere. As part of PRISM, Downey took on a leadership role, especially in the nonbinary and trans support group, and they became president their senior year.

"Giving people a space to exist and be accepted is really important," Downey said. "The people we have reached have been impacted by having this space."

Because of Downey's dedication to their research and fellow students, they received the Niccolai-Fustanio award as a rising senior and the Fugassi and Monteverde award upon graduation.

Downey graduated as part of the B.S.-M.S. program in chemistry. In fall 2024, they will attend the Max Planck Institute in Dresden, Germany to pursue their Ph.D. They said they hope the work they do will continue to shed light on questions in inorganic chemistry.

■ *Kirsten Heuring*



Alumni News

Recent Grad Applies Chemistry Lessons To Cosmetics Start-Up

Ananya Kapur has a colorful career.

As the founder and Chief Everything Officer of Type Beauty Inc. she is making waves in the world of cosmetics. Her New Delhi-based company has garnered mentions in Vogue, Elle and Harper's Bazaar for its inclusive approach to cosmetics that also address skin concerns.

"It's important to be super inclusive for every skin tone and skin type," said Kapur, who graduated from Carnegie Mellon University in 2021 with a bachelor's degree in chemistry and an additional major in business administration. "I have a deep love of chemistry, and I wanted to pursue it and business as well. With Type Beauty, my two areas of interest intersect in the most amazing way."

Her line includes 24 shades of foundation — the most of any Indian brand — that range from vanilla to cocoa and many variations in between. Each is available in formulas that help treat different skin issues such as acne prone skin, redness or fine lines.

Type Beauty semi-customizes makeup based on users' skin type and merges skin care and makeup in one product. The expanding, vegan makeup line includes concealers, foundations, primers, lip products, eyeshadows and tools, with more products in the works.

Type Beauty's team — about 30 people and growing — uses a scientific approach to create vegan and cruelty-free products. But before opening her own product lab, Kapur made her first lipstick in The Design and Making of Skin and Hair Products course taught by Teaching Professor of Chemistry Gizelle Sherwood.

"I love being in the lab. It's so fun to see something that you start from scratch and materialize into an actual product. For me that was a really big moment," Kapur said. "It was all really cool to learn."

Sherwood recalled Kapur during the cosmetics and hair product course. The course is taken by both chemistry and nonmajor students from across the university. In its current iteration, students learn about the chemical components in cosmetic products and the methods for preparing them. The course includes a hand-on laboratory experience. With regular guest lecturers from the School of Design, students also delve into marketing products.

"We knew Ananya's end goal was to open a business after graduation. It's been phenomenal watching her success," Sherwood said.

In 2024, Carnegie Mellon recognized Kapur as through Tartans on the Rise, which celebrates alumni who graduated in the last 10 years and are making an impact.

With more product launches on the horizon and a future artificial intelligence tool in the works, Kapur isn't slowing down anytime soon, and, with her Carnegie Mellon education, she's ready for what's next. She said being able to combine scientific training with business courses at Carnegie Mellon has been invaluable.

"It's really important to have a strong technical base in anything and to know the basics," she said. "There's so much you can do with that knowledge in any kind of industry."

■ *Heidi Opdyke*

Tartan Takes Flight

Carnegie Mellon University Class of 1980 alumna Janet Marnane knew she could have been happy in a research career using her Mellon College of Science chemistry degree.

There was just one problem: She really wanted to fly fighter jets.

“They were accepting women into the military academies when I graduated from high school, but what they were offering was not what I wanted to do,” Marnane said. “I’d always been interested in aviation.”

She saw her opportunity when a U.S. Navy recruiter showed her F-14 Tomcat aviator videos.

Lucky for her, a few years before her CMU graduation, the Navy opened the Flight Officer Program for jets.

Women were not yet allowed on aircraft carriers, but she still dreamed.

EARNING HER WINGS

In 1980, the Navy offered six openings nationwide to women interested in flight officer training school.

“I thought I didn’t have a chance,” Marnane said.

She applied — one of 23 applications in her region alone. But as one of five children growing up on a farm near Stamford, New York, Marnane was used to competition.

Months later, she was accepted into the 14-week program and moved to Pensacola, Florida.

“I was good at it,” Marnane said. “It was like drinking from a fire hose, but I had already been through that at Carnegie Mellon. Plus, it was something I really, really wanted to do.”

After completing flight officer training school, Marnane joined a training squadron and completed electronic warfare training. She learned how to operate the jet systems with a fleet replacement squadron. Finally, she was assigned to her first fleet squadron, Tactical Electronic Warfare Squadron Thirty-four (VAQ-34) with the mission of simulating enemy tactics for their own fleet’s training.

She said CMU prepared her for the military experience in several ways. A member of the swim team, Marnane was already fit and “aced the swim test” when she joined. She also valued diversity.

“In the CMU dorm, I lived on the floor with people from Ecuador, Pakistan and Iran and had roommates from Pittsburgh and Philadelphia,” Marnane said. “I didn’t think about diversity when I chose to go to CMU, but it was very cool to have that experience. It helped when I went into the military because people come from all over, all walks of life, all backgrounds.”

Photo courtesy of Embry-Riddle/Daryl Labello

UPWARD AND ONWARD

Throughout Marnane’s 25-year military career, women increasingly joined the Navy’s ranks. In 1993, Marnane received a call that the first two aircraft carriers were going to sea with women, and the air wing commander wanted her to join his staff. She became the first female officer to report to a carrier air group.

“I never went in thinking they were going to give me a hard time because I was a woman,” Marnane said. “I went in thinking I’m going to go in and kick butt, so that they couldn’t say, ‘Oh, you’re just here because you’re a woman.’”

For six months leading up to the launch, she led plans to accommodate women in the berths. It was a difficult challenge.

“I had detractors, but I also had champions,” Marnane said. “I had instructors and other people with whom I flew who insisted I get what I wanted because I deserved it.”

Once the carrier was at sea, Marnane lived her dream to the fullest.

“Being on the air wing staff, I flew with all of the squadrons: the F-14, EA-6B, S-3 and E-2,” Marnane said. “If you’ve seen ‘Top Gun,’ I’m Goose. I was either in the right seat or back seat doing the communications and the navigation, basically like a co-pilot.”

During her military career, Marnane rose to the rank of commander and served as an executive officer.

After retiring from active duty in 2006, she taught aviation-related subjects in the College of Aviation at Embry-Riddle Aeronautical University in Daytona Beach, Florida, until retiring in 2021.

“It has been a real honor to help break through some of the glass in the ceiling,” Marnane said. “Women still make up a very small portion of the aviation world. I’m happy to say I stay in touch with many of my former midshipmen and students, and the future is in very capable hands.”

■ *Ann Lyon Ritchie*

Collaborators in the Lab and Life

Anisha Gupta and Raman Bahal's first meeting was all about chemistry. But not that kind of chemistry — at least, not at first. The two met as undergraduates at Punjabi University, where they bonded over pharmacology and medicinal chemistry. They spent countless hours talking about the mechanism of diseases, the chemical structures of drugs and treatment regimens.

Over time, their friendship grew into something more. The couple, who earned their doctorates in Carnegie Mellon University's Department of Chemistry, married in 2008, and they still talk chemistry every day — as partners inside and outside the lab.

Bahal, associate professor in the Department of Pharmaceutical Sciences at the University of Connecticut, and Gupta, assistant professor of pharmaceutical sciences at the University of Saint Joseph, work at the intersection of nucleic acid chemistry and nanotechnology, designing and developing precision-based therapeutics to treat cancer and other diseases.

"We have been working together for a long time," said Bahal, who has co-authored 10 papers with Gupta. Together they have a combined publication list of nearly 80.

Their penchant for collaboration — and their interest in nucleic acid chemistry — blossomed as Ph.D. students. Bahal worked in the lab of Chemistry Professor Danith Ly, while Gupta, who joined the department one year after Bahal, worked with Bruce Armitage, professor and now head of the Department of Chemistry and co-director for the Center for Nucleic Acid Science and Technology (CNAST).

"It was an open-door policy with Danith's and Bruce's labs," Gupta said. "We had such a good collaboration there across their labs on the seventh and eighth floors of the Mellon Institute."

Ly is also a member of CNAST, an interdisciplinary community of scientists and engineers who explore the chemistry, biology and physics of DNA, RNA and gamma peptide nucleic acid (PNA). PNAs, synthetic nucleic acids containing the same base pairs as DNA and RNA but with a protein-like backbone, are versatile molecules that can be designed to bind to specific DNA and RNA targets inside cells to alter the expression of disease-causing genes and, ultimately, the course of disease.

With their backgrounds in pharmacy and medicinal chemistry, Bahal and Gupta recognized PNAs' therapeutic potential and dug in — first with a deep dive into PNA chemistry at Carnegie Mellon and then with an exploration of how to deliver the PNA into diseased cells at Yale University, where they worked as postdoctoral researchers.

"We collaborated with Yale's Department of Biomedical Engineering to formulate PNAs into nanoparticles, which opened up many different avenues," Gupta said. "You can change the formulation to see how the delivery changes, you can tweak the amino acid on the PNA backbone and change its chemical properties. The possibilities are limitless."

Bahal and Gupta often work hand in hand as their respective labs design and develop PNAs and other nucleic acid-based molecules to target brain cancer and lymphoma, liver disease, and stroke. Designing a PNA is only the beginning. They are also developing delivery methods to get the PNAs to the target cells and testing PNA packages in preclinical models.

"When you think about bringing a therapeutic candidate from bench to bedside, there are a lot of components there: disease biology, chemistry, delivery," Bahal said. "With PNA chemistry, there's a lot of hidden treasure, and we're trying to find out if we can connect some of those dots."

Recently, Bahal used a modified gamma-PNA to target oncogenic DNA, a root cause of cancer. Bahal's gamma-PNA successfully inhibited the expression of the c-Myc oncogene, which is implicated in various cancers, from multiple myeloma to breast cancer. He has also discerned that PNA can be used as a combination therapy for cancer treatment. Bahal's research showed that treating brain tumors in a preclinical model with gamma-PNA first can sensitize tumors to temozolomide, which is a drug of choice for brain cancer.

He's working to patent the various gamma-PNA technologies being developed in his lab and is talking with venture capitalists to potentially license the technology or launch a startup, with the goal of bringing it to patients. For his work, he received the 2024 RNA Society Moderna Award for Biomedical Innovation in RNA, the 2023 Oligonucleotide Therapeutic Society Young Investigator Award, and he was recently elected a senior member of the National Academy of Inventors. Gupta's work was also recently recognized with the 2022 American Association of Colleges of Pharmacy New Investigator Award.

Finding a good therapy that can increase a patient's life or their quality of life has been a driving force for Bahal and Gupta since their undergraduate days. Initially, they planned to work in the pharmaceutical industry, but they credit Armitage and Ly for motivating them to consider academia.

"I feel so lucky to have had such close mentoring — the time that both professors would invest in their students and how they would sit down and talk to us and coach us," Gupta said.

Bahal agreed.

"We were international students. We came from India, leaving our families behind," Bahal added. "Danith and Bruce were so supportive. Even now, when we meet Bruce or Danith at a conference or somewhere, it feels like meeting someone from home."

With two young children at home, dinner-table conversations these days tend to revolve more around what's happening in elementary and middle school. That's not to say that Bahal and Gupta still don't talk shop.

"DNA and PNA are two words that my daughter picked up when she was little," Gupta said.

"I was a little concerned," Bahal joked. "She should probably start with ABC first rather than going directly to DNA."

It may turn out that chemistry is a true family affair.

■ *Amy Pavlak Laird*

REQUEST AN

Alumni Dinner

Oles Isayev met with Lindsey Pherribo (MCS 2013) and Marcia Bent Henry (MCS 1984) in New Orleans to discuss the latest developments in the Chemistry Department and Mellon College of Science, including the construction of the Richard King Mellon Hall of Sciences and the Carnegie Mellon University Cloud Lab.

Chemistry Head Bruce Armitage met with alumni for a dinner in Menlo Park, California, on Aug. 17, 2023.

Robin Anwyl (MCS 2021) and Theodore Warner (MCS 2021) joined in the Bay Area dinner.

Interested in requesting a dinner in your area?

Contact Mitch Coates at mitchelc@andrew.cmu.edu or at 412-370-3931.

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