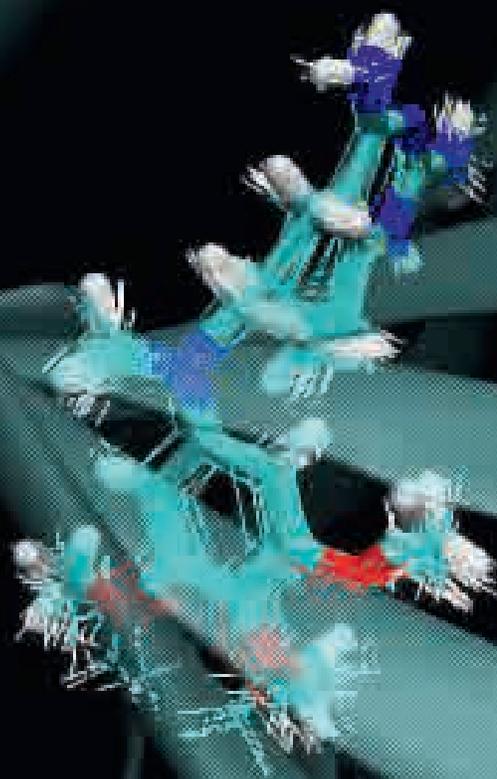




ILLINOIS INSTITUTE OF TECHNOLOGY

CHEMISTRY ELEMENTS

A Publication of the Department of Chemistry at Illinois Tech



Fall 2020



Welcome to the eighth annual issue of *Chemistry Elements*. I want to start off this letter by first thanking our faculty for their outstanding job changing over to online teaching, of both lectures and labs, when the shutdown was announced in March due to the COVID-19 pandemic. This was a very challenging new way to teach. They are to be recognized for their dedication and success given these unprecedented circumstances. Our department came through well. Additionally, our research-active faculty quickly stepped up to adopt the new research lab protocols, and we have managed to keep things running smoothly and safely. Thanks also to our students who adapted to online instruction. Another round of applause is due to our alumni, students, faculty, and staff who participated in our first-ever virtual end-of-the-academic-year party and award ceremony at the end of April. Our graduating students had a virtual commencement in May, as you may know. These have been challenging times indeed. To help bring back campus fun while some of us are back on campus, we held a socially distanced outdoor pumpkin carving event and a department contest for Mole Day for students in October.

Illinois Tech was recently recognized as No. 1 in the Chicago region for occupational earnings power by The Brookings Institution and No. 39 Best Value University in *U.S. News & World Report*. For these reasons and many more, we are working hard to promote our undergraduate programs, along with our graduate ones, to bring an excellent educational tradition and relevant

Letter from the Chair

opportunity to our young chemists. We have solicited our very own Chemistry Alumni Ambassadors who will help us with local area high school recruitment at their respective schools, as well as career counseling for our prospective students. While we continue to have a larger incoming undergraduate population in recent years as compared to previous years, we are determined to focus on building our undergraduate programs even more.

Many thanks to Bob Frey (CHEM '65) for creating the Robert E. Frey Jr. Endowed Term Chair in Chemistry, which was awarded to Associate Professor David Minh. Congratulations to David for achieving the first endowed chair position in the Department of Chemistry's recent history.

We want to also thank alumnus Ted Brown (CHEM '50) for initiating the Illinois Institute of Technology Chemistry Graduate Fellowship. This fellowship helps attract new Ph.D. students, especially those who are dedicated to teaching. We look forward to more gifts to expand the breadth of this fellowship. We were able to bring in eight new Ph.D. students this fall, two of whom are participating overseas until they can get to campus.

Congratulations are due to Katie Leight, who was promoted to senior lecturer and became associate chair in January. Katie brings a lot of energy and ideas to the department in her new role and is well-liked by the students. She is currently leading our Chemistry Club to deliver virtual presentations to local high schools and community colleges for promotional purposes. Katie also helped initiate our Summer Scholars program that hosts high school and community college students who participate in research projects with our research labs. Thanks are due to Ben Zion for his three and a half years of dedicated service as associate chair. He continues to teach, advise students, and manage our department's instrumentation.

Congratulations to our Assistant Professor Jean-Luc Ayitou, who was named a Researcher to Know for 2020 by the Illinois Science and Technology Coalition (ISTC) for his work in organic and photochemistry, in addition to being elected vice chair of the Argonne National Laboratory Center for Nanoscale Materials User Executive Committee. One of his students, Ph.D. candidate Young Ju Yun, was not only voted in as the 2020–21 Kilpatrick Fellow, but received the Starr/Fieldhouse Research Award to pursue collaborative work at Argonne National Laboratory. Congratulations also to two other faculty

members: Professor Joy Chong received a four-year National Institutes of Health grant for her project titled "Development of Superior Chelation Chemistry for 89Zr-ImmunoPET Imaging," and Assistant Professor Andrey Rogachev received an ACS-PRF (Petroleum Research Fund) grant award for his work titled "Deep Understanding of Catalytic Activity through High-Level Calculations."

Due to the pandemic, we had to postpone the 39th Kilpatrick Lecture to a future date—stay tuned.

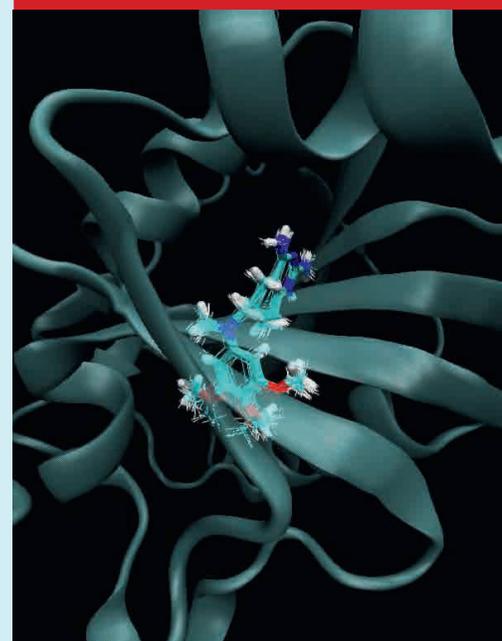
As an African proverb says, "Smooth seas do not make skillful sailors." It's the hard knocks in life that shape us into something stronger, wiser, and more resilient. We are getting through this tough time together. We hope all is well with you and your families. We want to thank you for your continued support and loyalty.

I wish you a happy and healthy 2021!

Yuanbing Mao
Professor and Chair
Department of Chemistry

December 2020

COVER: Conformations of a small molecule bound to a rigid protein (ribbon). Image created by Associate Professor of Chemistry David Minh's computational chemistry research group.





Chemistry's David Minh Launches Machine Learning Research Through New Chair Position

by Linsey Maughan

Associate Professor of Chemistry David Minh has been named the inaugural Robert E. Frey Jr. Endowed Chair in Chemistry, a five-year position that will enable Minh to expand his computational chemistry research in a new direction by applying machine learning to chemistry.

The creation of the chair position is the result of a donation from Frey (CHEM '65), an alumnus whose contributions in support of the university also include funding the remodeling of the chemistry department's office suite. Among its benefits, the new chair position offers Minh \$40,000 per year in research funding, which he says will primarily pay the salary of a research scientist to help support his new project.

Minh joined the faculty in the Department of Chemistry in fall 2013. His research at Illinois Institute of Technology has focused on computational chemistry.

"The main focus of my group is in developing new computational methods to predict how tightly small molecules bind to proteins," Minh says. "We also model how proteins move and interact with small molecules, working closely with experimental groups to better understand how biological systems work. Our work has implications for drug and protein design."

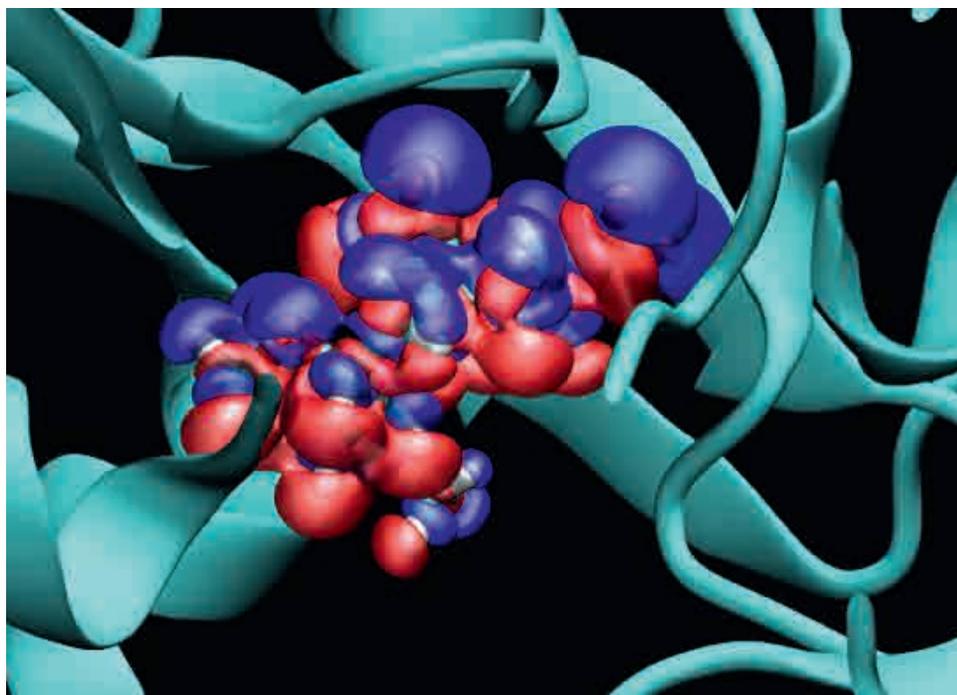
Minh is excited to now explore machine learning, a process that is increasingly being applied in chemistry research and utilizes data to inform predictions.

"I am aware of work in which machine learning has been used to predict the products of a chemical reaction; reaction conditions—such as solvents, catalysts, and temperature—that optimize the yield of a reaction; quantum mechanical ground-state energies; and binding affinities of protein-ligand complexes," Minh says. "I would like to predict how small organic molecules are polarized when binding to proteins. This could affect how tightly they bind and whether a molecule could be a drug."

As a precursor to his new research, Minh and his colleagues also published a paper in 2020 in *Physical Chemistry Chemical Physics* titled "On the Polarization of Ligands by Proteins."

"In this paper we used mixed quantum mechanics/molecular mechanics calculations to see how much small molecules are polarized by their protein environment," Minh says. "Part of what I have proposed to do as Frey chair is to perform similar calculations using fast machine-learning approaches rather than computationally expensive quantum chemistry calculations."

Differences in electron density around a small organic ligand embedded in a protein (3fv1 in the protein data bank) opposed to the gas phase. Blue and red contours illustrate the gain and loss of 0.0005 Bohr^{-3} of electron density.





Device Characterization of Dye Sensitized Solar Cell.”

In the award letter, Vice Provost for Research Fred Hickernell writes that this project “takes advantage of Ayitou’s recent work on synthesis of a dye that exhibits an excited electron state that is a triplet exciton.”

“Such an exciton has a much longer lifetime and thereby may be suitable to enhance the conversion efficiency of dye sensitized solar cells,” Hickernell writes. “This is an important advancement if successful, with potential commercialization.”

Students involved in this project will be trained in organic synthesis and photovoltaic device fabrication. This is an interdisciplinary effort involving the Department of Chemistry and the Department of Mechanical, Materials, and Aerospace Engineering at Illinois Tech.

Ayitou Named ISTC Researcher to Know

The Illinois Science and Technology Coalition (ISTC) named Assistant Professor Jean-Luc Ayitou as a Researcher to Know for 2020 for his work in organic materials and photochemistry. His lab pursues the creation of novel organic chromophores for applications ranging from solar energy to sustainable chemical syntheses.

The ISTC is a “member-driven nonprofit that measures, connects and advocates for the state’s research and innovation community.” The Researchers to Know list is released annually in conjunction with the R&D issue of ISTC’s *Illinois Innovation Index*. This recognition places Ayitou among a stellar group of leading researchers across the state of Illinois.

The ISTC held a virtual event in September 2020 for their announcements, bringing together university and industry professionals, startups, nonprofits, and government officials interested in scientific research and commercialization. As stated in the award letter from ISTC, this recognition “should amplify Ayitou’s research efforts and bring him closer to his goals for environmental chemistry and converting solar radiation into useful energy.”

Ayitou was also awarded an Educational and Research Initiative Fund from Illinois Institute of Technology’s Office of Sponsored Research and Programs for his project proposal, “Solar Energy Conversion Using Triplet Excitons: Synthesis and



Congratulations to Katie Leight

Katie Leight was promoted to senior lecturer and associate chair in January 2020. She also manages the organic chemistry labs. Leight joined the department in fall 2017 after receiving her Ph.D. in chemistry from the University of Arizona.

Summer Learning Program for Chicago Public School Teachers

Chicago Public Schools elementary and middle school science teachers were linked with Illinois Tech scientists and engineers in August as part of a collaboration with the Academy for Urban School Leadership (AUSL) and National Louis University (NLU).

Associate Professor Adam Hock ran a module with biology graduate student Mohsin Ishaq titled “Density—Not Just for Boats and Rocks!” This event stemmed from a collaboration between Illinois Tech, AUSL, and NLU, which received a U.S. Department of Education Teacher Quality Partnership Grant and brought in Illinois Tech as a subcontractor.

ACHM Program Affiliates Gather at PITTCON 2020 and Axion Labs

Affiliates of the Illinois Tech Analytical Chemistry program (ACHM) attended Pittcon (Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy), which took place from March 1–5 in Chicago. The group also gathered after the conference on March 2 at Axion Labs, located in Chicago, for an event hosted by Lee Polite, president of the company. Present were: Cody Beaumont, senior director of research and quality control, Doterra Inc.; Mary Ellen McNally, global R&D technical fellow, analytical sciences, FMC Corporation; Brian Leaf, director of analytical R&D at Teva Pharma; Diep Nguyen, ACHM program director; Yuanbing Mao, Department of Chemistry chair; ACHM student Joseph Lustig; alumna Ilana Lemberger (M.A.S. ACHM ’13); and Amandeep Sandhu, assistant professor in the Institute for Food Safety and Health at Illinois Tech. Beaumont, McNally, and Leaf are members of the ACHM Industrial Board. Polite is an adjunct instructor in the Department of Chemistry.



Lee Polite talks to ACHM members at his company, Axion Labs, Inc.



[Left to right] Mary Ellen McNally, Yuanbing Mao, Joseph Lustig, Ilana Lemberger, Cody Beaumont, Brian Leaf, Diep Nguyen, Lee Polite, and Amandeep Sandhu.

'Green Chemistry' Research Exploring Possibility of Using Water as a Solvent

by Linsey Maughan

New research underway in Assistant Professor of Chemistry Jean-Luc Ayitou's AJA Laboratory explores the feasibility of using water as a solvent, a "green chemistry" project that, if adopted in industrial settings, could

have a positive impact on the environment.

Will Blodgett (CHEM, CHE, M.S. CHEM 4th Year), a chemistry and chemical engineering double-major who is enrolled in the accelerated master's degree program in chemistry, is leading the project. Blodgett, whose passion since high school has been environmental-based science, became Ayitou's advisee after discovering his professor's work in the areas of green chemistry and photochemistry.

"Organic chemistry, which Professor Ayitou introduced me to during my freshman year, became one of my favorite subjects," Blodgett says. "I talked with him after class early on in the semester, when he introduced me to the organic-water biphasic project, the principles of green chemistry, and his interest in photochemistry. It all aligned perfectly."

As Ayitou describes it, green chemistry protocols "aim at mimicking Mother Nature with an emphasis on reducing chemical wastes downstream." They are "an integral part" of the research projects underway in Ayitou's lab, he says.

Blodgett spent two years preparing for the biphasic project with support from his lab partner, Alysia DeSimone (CHE, M.S. ENVE 4th Year). Their initial testing with milliliter scales was "very promising," Ayitou says. This fall Blodgett has begun testing large-scale reactions to using water as a solvent in order to gauge the feasibility of

following the same protocol in industry settings.

"Water cannot be used to dissolve many organic compounds, leading many industries to use large amounts of organic solvents, which are more harmful to the environment," Blodgett says. "With the addition of phase transfer nanocavities in water, we are able to use a much smaller amount of organic solvent."

After the research is complete, Ayitou and Blodgett hope to publish their findings. Ayitou says he is confident the biphasic reaction technique will prove viable alongside other green chemical synthetic processes.

"We hope to integrate this new approach with existing green chemistry techniques to raise awareness for environmentally benign synthetic protocols," Ayitou says. "These can be implemented in the industry in order to minimize the use of toxic reagents or to reduce toxic waste."



Illinois Tech student Will Blodgett (CHEM, CHE, M.S. CHEM 4th Year) works in Assistant Professor of Chemistry Jean-Luc Ayitou's laboratory.

Chemistry Students Visit Nalco Water Chemical Industry Company

On February 4 Illinois Tech chemistry students visited the R&D lab of Nalco Water, an Ecolab company located in Naperville, Illinois. Nalco is a supplier of water, energy, and air improvement solutions and services. Another entity is Nalco Water University, a unique, high-tech learning environment dedicated to developing expertise to minimize water usage. They were hosted by Francois Battlo, R&D director at Nalco, who arranged a tour that included an exhibition room with equipment, photos, samples, and ideas. The students were introduced to the heat/cool water system and related detection methods for water components. They viewed a research work area with XRD, RAMA, UV-Vis, microscopy, HPLC, and ICP-MS, among other instrumentation. Thank you to Battlo for hosting this informative visit, giving insight into a career option for chemists.

Environmental Chemistry Off to a Good Start

This fall Professor Yuanbing Mao taught CHEM 472: Environmental Chemistry, the department's first environmental chemistry course offered in recent years. As part of the course, Mao hosted two fellows from the Metropolitan Water Reclamation District of Greater Chicago: Ali Oskouie, senior scientist, and Joseph Kozak, supervising environmental research scientist. Kozak gave a talk entitled "Wastewater 101" and Oskouie presented "Water Chemistry and Wastewater." Illinois Tech has a longstanding collaborative relationship with the Water Reclamation District.



Chong Receives NIH Award

Professor Hyun-Soon "Joy" Chong received an award for her research titled "Development of Superior Chelation Chemistry for 89Zr-ImmunoPET Imaging" from the National Institutes of Health (NIH/1R01EB029800-01A1). This is a four-year grant with the current award totaling \$403,933. This is a notable achievement for Chong, who has consistently gained funding from the NIH in past years.

Assistant Professor Jean-Luc Ayitou was elected as the vice chair of the Argonne National Laboratory Center for Nanoscale Materials User Executive Committee. The Center for Nanoscale Materials (CNM) User Executive Committee (UEC) "serves as an advocacy group for the CNM and its user community, provides advice to the CNM Director on matters affecting the user community, and ensures good communication between the CNM user community and CNM leadership. The CNM-UEC is also responsible for organizing the scientific content of the annual joint Advanced Photon Source (APS)/CNM Users Meeting."



**Congratulations to Our
2020-21 Kilpatrick Fellow**
Young Ju Yun, Ph.D. Candidate

**Yun Receives 2020 Starr
Fieldhouse Award**

Young Ju Yun, Ph.D. candidate and research assistant in Assistant Professor Jean-Luc Ayitou's lab, is the recipient of the 2020 Starr/Fieldhouse Award from the Office of Research at Illinois Tech. Her proposal, "Energy Upconversion Using Organic Donor-Acceptor Dyads: Synthesis and Photophysical Characterization of the Dyads," featured a strong research plan to collaborate with the Center for Nanoscale Materials at Argonne National Laboratory.

Yun also received a third place poster presentation award at the second Frontiers in Photochemistry Conference held in February in Nassau, Bahamas.



Students guessed at the number of moles in this flask to win the ACS stuffed "Professor Molarity" for Mole Day, October 23.

Influit Energy Startup Co-Founded by Chemistry's Elena Timofeeva Wins DoD Ventilator Contract

by Linsey Maughan

A local startup co-founded by Illinois Institute of Technology Professor of Physics Carlo Segre, Research Associate Professor of Chemistry Elena Timofeeva, and two-time physics alumnus John Katsoudas (PHYS '97, M.S. '04) has been awarded a contract with the United States Department of Defense to produce low-cost ventilators in response to the COVID-19 pandemic. The startup, called Influit Energy and founded in 2014, develops flow batteries made with nanofluids. Katsoudas serves as chief executive officer; Segre is the chief technology officer; and Timofeeva serves as chief operation officer and director of research.

The ventilator concept was developed by Katsoudas this past spring.

"COVID-19 hit and then there was a ventilator shortage," Katsoudas says. "They're not that complicated, so I thought



the supply chain would catch up—and then the supply chain wasn't catching up. There was this call out to the auto industry to start making [ventilators]. I said to myself, why don't we just build a ventilator? It's nowhere near as complicated as the things that we do day to day."

Katsoudas submitted his design to a hackathon hosted by mHUB, a Chicago-based

incubator that exists to support local makers and startups. He then began assembling a team of technical experts to move the project forward regardless of the competition's outcome. After winning first place in the hackathon, Katsoudas and 20-plus volunteers spent three weeks assembling a benchtop prototype. The ventilator design is open-source and license-free, making it is easy to reproduce at a far lower cost than market models. The parts needed to build the ventilator are widely accessible.

After completing the prototype, Katsoudas submitted the design to a Department of Defense solicitation to develop ventilators and was recently awarded a \$1.7 million contract to fund the design's refinement and commercialization. The contract will begin on December 1, 2020.

"After the mass-producible device and its quality-management systems are mapped out, the first five

ventilators will be submitted for testing by month 10 of the project, and the entire value supply chain will be Food and Drug Administration approved within a year," Katsoudas says. "I hope this design will be sufficiently low cost to disrupt the existing supply chains and force a change on how these critical medical devices are made available to lower-income communities and the developing world."

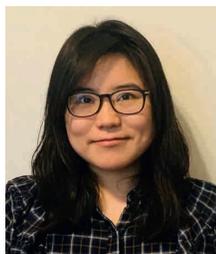


2019–20 Graduate Student Awards



Teaching Assistant Award

Damola Taye Shuaib



Chemistry Department Service Award

Young Ju Yun

2019–20 Undergraduate Student Awards



Junior Award

Aaron Gregory



Senior Award

Ashton Dato

Kilpatrick Tuition Scholarship Awards



William Blodgett



Victoria Sabo



Abigail Schulz

2019–20 Degree Recipients

Bachelor of Science in Chemistry

Ashton Dato, Keara Rigg, Abigail Schulz, Andrew Shahidehpour

Master of Science

Nouf Safar H. Almotari, Nalah Alqahtani, Dana Alramahi, Khawlah Hamad A. Alzahid, Hanyin Zhang, Shuyao Zheng

Master of Science in Analytical Chemistry

Megha Chandrashekha, Wai Cheung, Kristin DeAngeles, Teresa Di Dio, Meagan Eggebeen, Jordan Fritz, Elisabeth McKenna, Jansen Seheult, Michelle Workman

Certificate—Regulatory Science

Marsha Bures

Master of Chemistry in Materials Chemistry

Karla Torruellas

Doctor of Philosophy

Shuyang Liu (Adviser: Andrey Rogachev), Elahe Moazzen (Carlo Segre), Golbarg Mohammadiroozbahani (Xiyun "Richard" Guan), Siyuan Ren (Hyun-Soon "Joy" Chong), Yunjie Xu (Adam Hock), Youwen Zhang (Xiyun "Richard" Guan), Yiqing Zhao (Adam Hock)

Become an Alumni Ambassador for Illinois Tech Chemistry!

Dear Illinois Tech Chemistry Alum,

I hope that you and your family are all staying well during this very challenging time.

As the chair of the Department of Chemistry, I am writing today in this time of need to encourage you to become an Illinois Tech Chemistry Alumni Ambassador. With your Scarlet Hawk pride, passion, and love, here are a few more formal ways to give back by dedicating your precious time to us:

1. **Communicating with admitted chemistry students in your area (by in-person or virtual meeting, phone call, etc.)**
2. **Referring prospective students to the chemistry programs at Illinois Tech**
3. **Attending regional college fairs and visiting high schools in your area**

As you may have heard, Illinois Tech has seen a decrease in our international graduate student enrollment at present, and now—more than ever—we need to increase our undergraduate population, including in the Department of Chemistry.

By meeting with high school students, you can share your campus memories and give examples of how your Illinois Tech education prepared you for your career. An Illinois Tech Chemistry Alumni Ambassador can affect prospective students in a meaningful and personal way, making a dramatic difference in our enrollment.

Another way to serve as an Illinois Tech Chemistry Alumni Ambassador is to offer career counseling for our current students and help them navigate the highly complex and competitive job market. You can help us educate them about your industry and share some of your professional experiences.

Help us to get our special equation across to prospective undergraduate chemistry students: big city + small intimate class setting = successful students!

We hope you will join our chemistry campaign. We would very much appreciate your generosity by giving your time and sharing your enthusiasm for chemistry and an Illinois Tech degree. I look forward to hearing from you soon—please do not hesitate to reach out. When you contact me, I will recommend you to our Office of Undergraduate Admission for becoming an Illinois Tech Admission Alumni Ambassador (<https://admissions.iit.edu/undergraduate/alumni>). In this way, you will be additionally:

- i. **Attending Undergraduate Admission events throughout the year**
- ii. **Staying updated with a bimonthly newsletter from the Alumni Association**
- iii. **Becoming part of the formal organization, which recruits the future alumni who will continue the traditions of Illinois Institute of Technology**
- iv. **Joining Alumni Chapters to stay connected with Illinois Tech in multiple ways**

Best regards,

Yuanbing Mao
Professor and Chair
Department of Chemistry
ymao17@iit.edu

Chemistry Pumpkin Carving October 2020

