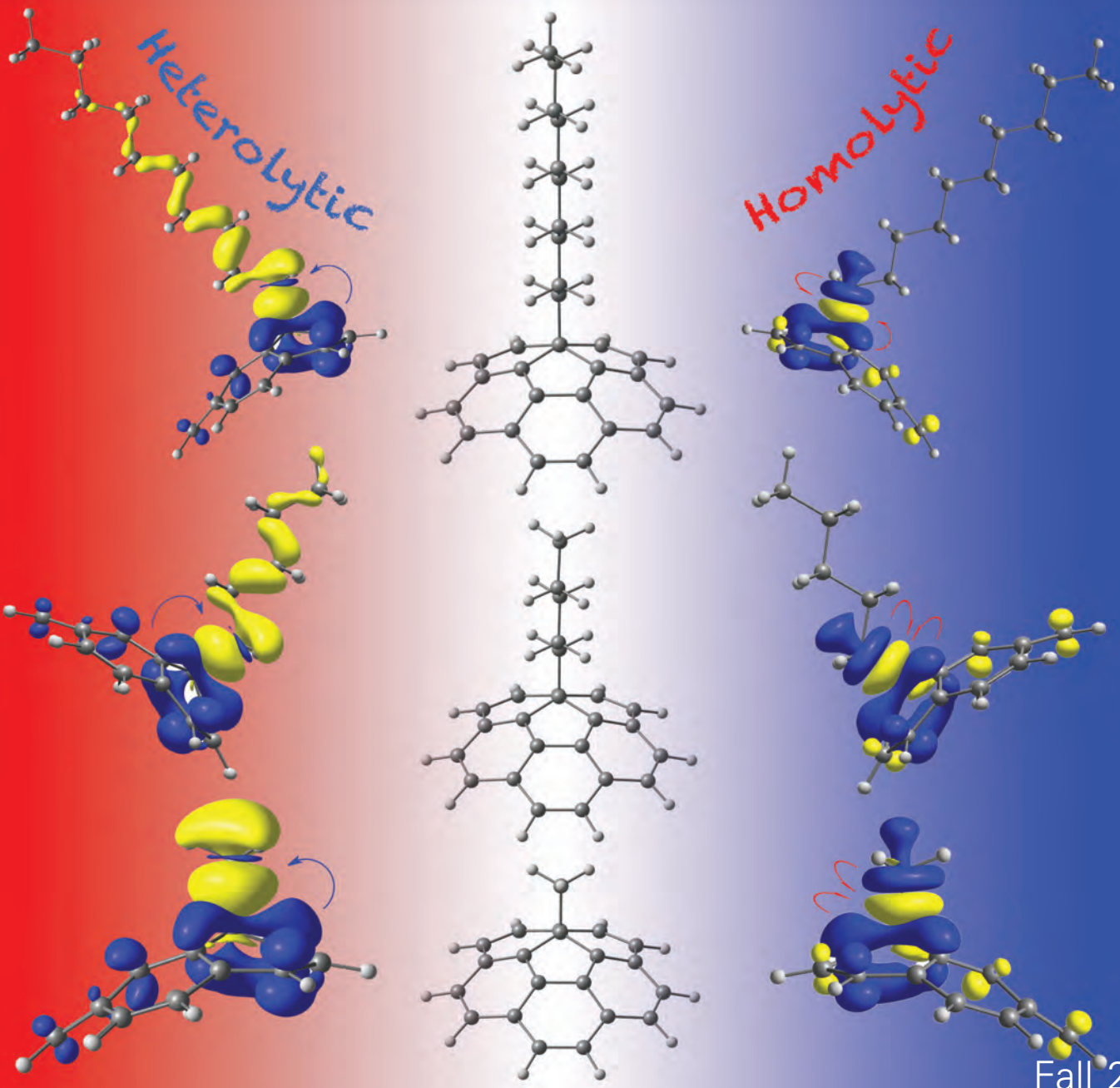
ILLINOIS INSTITUTE OF TECHNOLOGY

CHEMISTRY ELEMENTS

A publication of the Department of Chemistry at Illinois Tech

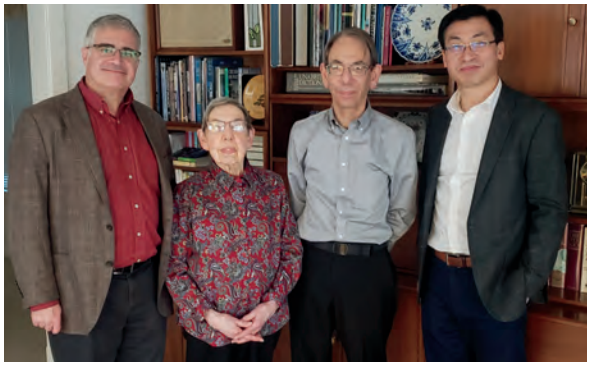


Fall 2019

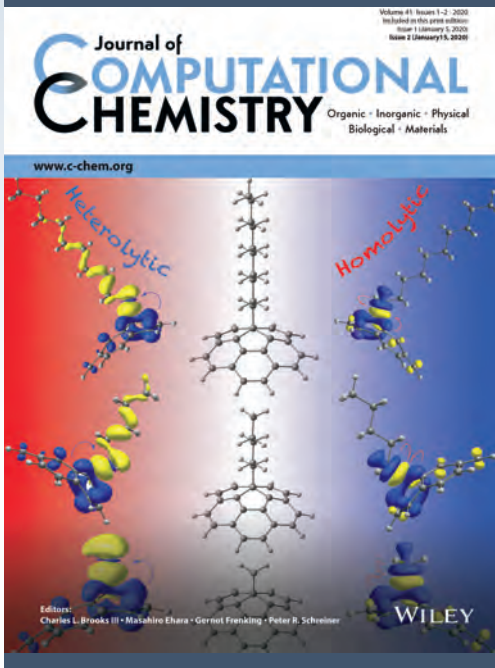
Thank You to the Fanta Family!

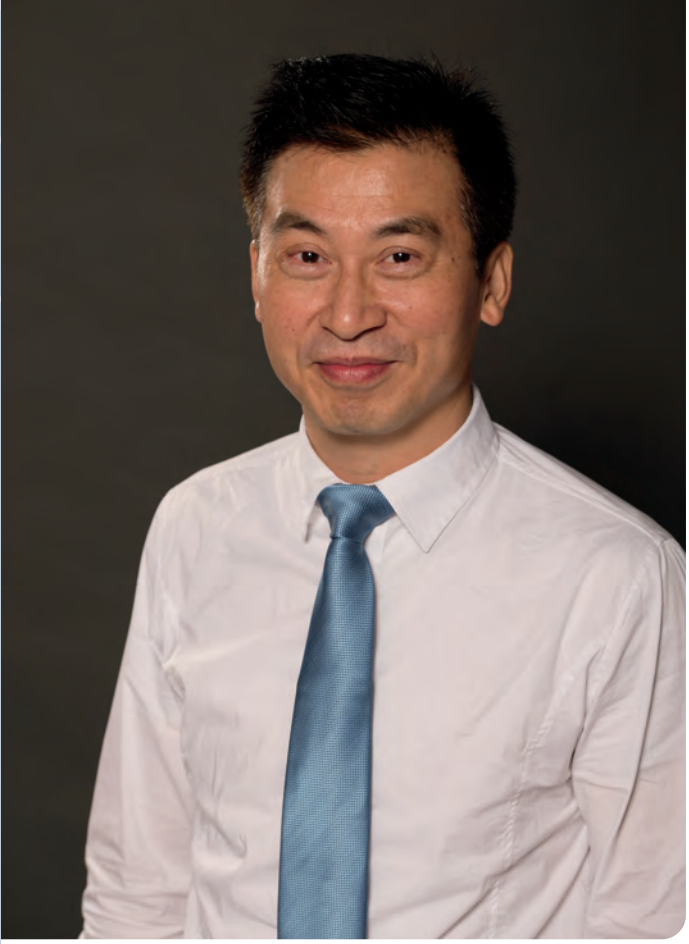
Professor Yuanbing Mao and College of Science Dean Lance Fortnow met with members of the Fanta family in December. The Fanta family has generously decided to continue their support for chemistry graduate students.

The new endowed fellowship is in honor of Paul E. Fanta, who was a professor in the Chemistry Department from 1948-1984.



COVER: Image created by Jingbai Li, Ph.D., in the Rogachev group depicting a competition between homolytic and heterolytic mechanisms, the subject of which was published in *J. Comput. Chem.*, 2020, 41, 88–96.





Letter from the Chair

Welcome to the seventh annual issue of *Chemistry Elements*. I am very happy to be a part of Illinois Tech and the Department of Chemistry.

First, I wish to thank Professor Carlo Segre for his three-year service as interim chair. He leaves the department in an organized and fine state, having implemented numerous improvements for both faculty and students. His efforts to advance the instrumentation and research capabilities in the department have resulted in the acquisition of a high-resolution X-ray absorption spectroscopy system and a thermogravimetric analyzer.

During the first month in my new role, I met with our undergraduate chemistry majors, graduate students, and faculty, asking for comments and suggestions. This has proved interesting and fruitful—insights into a number of areas where we are not only successful, but in which we can improve and grow were provided. I also look forward to setting up interdepartmental collaborations. For example, I visited the Institute for Food Safety and Health (IFSH), and met with colleagues from Illinois Tech's Office of International Affairs.

My vision for the Department of Chemistry within the next five years can be summarized as *Vision 1-2-3*:

1) To have our department ranked in the top **100** in *U.S. World & News Report* through ongoing support and collaborations both outside and within the department

2) To motivate our entire department to **double** our research enterprise in terms of proposals submitted, journal publications, presentations given, and active grants

3) Pledge to **triple** the department's overall undergraduate enrollment. Illinois Tech President Alan W. Cramb recently announced that our most recent class of first-year students is one of the largest in university history. Our department's undergraduate enrollment for the fall 2019 semester was the highest we have seen in years, due to our active outreach effort and five new bachelor of science programs created in 2017. This increase follows the guidelines set forth in the new Illinois Tech Strategic Plan led by Provost Peter Kilpatrick. We are actively working on outreach endeavors, especially in the surrounding Chicago area by reaching out to local high schools and community colleges to promote our programs.

   Through these collective initiatives and effort, I think there is much we can accomplish, and everyone agrees that increasing enrollment is the most important priority.

In other news, our American Chemical Society club is looking forward to manning its own booth at the chemistry event to be held at Northwestern University in October with a theme of "Marvelous Metals." I have met with our chemistry club officers—they are a serious and engaged group of students.

At the time of writing this letter, we are looking forward to the 2019 Reunion Weekend this month. Meeting with chemistry alumni is also a priority of mine, here on campus or as I travel to conferences and meetings.

On the research front, 70 percent of our research faculty are funded by external grants and many are working on multiple projects. I am pleased to report that Professor Rong Wang received a three-year National Institutes of Health award to continue working with her medical collaborators. Associate Professor David Minh was awarded a National Science Foundation grant in collaboration with Associate Professor of Applied Mathematics Lulu Kang. Chemistry faculty earned two internal 2019 awards from the Wanger Institute for Sustainable Energy Research.

Members of the department were very sorry to hear of the passing of Professor Emeritus Robert Filler in January 2019. Filler served as a chemistry professor, department chair, and college dean during his time at Illinois Tech. He was well-known for his research in the area of fluorine chemistry.

Please keep us in mind if you are in the Chicago area or if you plan to attend an ACS meeting. We always welcome communication from our alumni, whether that's to share your thoughts and memories or offer ideas and suggestions.

I wish you a happy and healthy 2020!

Yuanbing Mao
Professor and Chair
Department of Chemistry

September 14, 2019

New Chair Brings Expertise in Materials Chemistry and Nanoscience

Scaling metal oxides to a nanoscale dimension substantially alters phase stability and interfacial activity with tremendous manifestations of unique physical phenomena. Developing novel nanostructured metal oxides with an understanding of their synthesis-property-application relationships has paramount importance to meet the materials needs and challenges of our evolving society. The Multifunctionalized Applications of Oxide (MAO) Research Group designs advanced nanomaterials, achieves desirable properties and functionalities, and tackles complex interdisciplinary material challenges. Studies focus on developing facile, green, and reliable synthesis methods for complex metal oxide nanomaterials, as well as investigating their novel properties and application potential in the areas of optoelectronics, energy conversion, and sustainability. Specifically, the MAO Group conducts research in three areas of materials chemistry and nanoscience.

Luminescent Materials

Solid-state lighting sources by phosphor-converted white-light-emitting diodes (pc-WLED) play an important role in general indoor and outdoor lighting, traffic signals and automobiles, architectural decoration, and horticultural lighting, among others. Central to the performance, cost, application, and prospects of pc-WLEDs are the type and quality of phosphors used. Developing new, desirable phosphor candidates is a daunting task, with various materials and technical parameters to consider and balance. The MAO Group investigates and develops nanostructured, complex metal oxide phosphors by complementary techniques—especially X-ray spectroscopies—to determine their electronic structure. This is a critical step in learning how to control, design, and engineer these oxides. The MAO Group targets the applications of luminescent materials for lighting, radiation detection, biodiagnostics, thermometry, sensing anti-counterfeiting, and plant cultivation. Through research, discovery, and development of nanostructured luminescent materials, existing and emerging applications in optoelectronics, sensing, and health care diagnosis and treatment will be expanded.

Photoelectrochemical Catalysts for Sustainable Technologies

Cost-effective clean energy requires the exploration of new materials and/or structures as efficient electrodes for industry-level photoelectrochemical (PEC) water-splitting, carbon dioxide reduction, nitrogen fixation, etc. Splitting hydrogen from oxygen in water molecules produces hydrogen fuel with only water as the by-product. To meet urgent and critical needs confronting the sustainable energy-powered economy, the MAO Group is developing active and efficient electrocatalysts from earth-abundant materials for water electrolysis. They focus on types of strongly-correlated complex transition metal oxides, e.g. delafossite oxides $Cu^{I}M^{III}O_2$. Mao and his students study the underlying mechanisms and parameters governing water-splitting reduction/oxidation activities and ideally discover convenient activity descriptors. As nanomaterials outperform their bulk counterparts because of increased interacting sites due to shorter lateral diffusion distance and lower reflectivity, the MAO Group is interested in assembling nano-building blocks for more desirable structures—realizing higher performance and better functionality by exploiting new scaling and hierarchical laws. For example, Mao and his students have explored zinc oxide nanostructures, such as nanowire arrays, nanoforests, and an interconnected caterpillar-like network. These unique nanoarchitectures enable an impressive water-splitting performance, opening a promising road ahead governing desirable three-dimensional nanostructures, and broadening the application potential of 3D nanotechnology from both minimized functionality to large-scale industrial devices. These 3D nanostructure innovations are expected to open other related fields of nanoscience and nanotechnology to benefit the entire energy storage and conversion field.

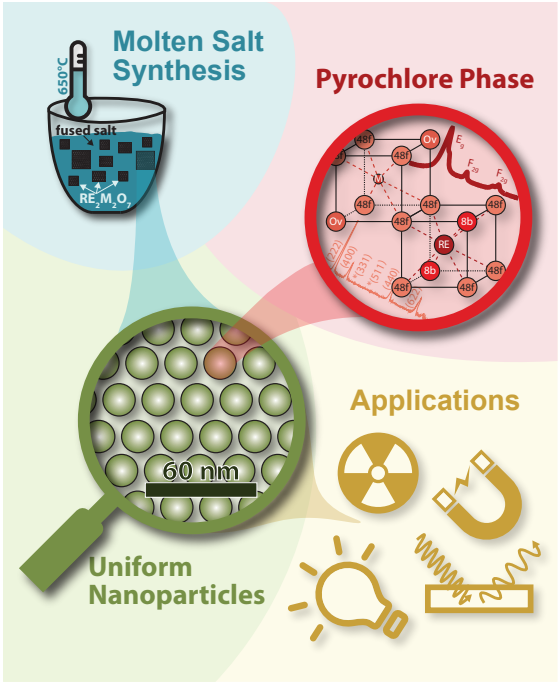


Figure 1: Schematic representation of homogeneous complex metal oxide nanoparticles synthesized by a molten-salt synthesis method with applications in the areas of solid-state lighting, scintillation, magneto-optics, and nuclear waste remediation, etc.

Nanotechnology for Water and Agriculture

Water has become a major topic of interest worldwide, as its uncontaminated form is becoming scarce in some countries. Responding to the resulting challenges of sustainable development and food and agriculture requires new and impactful technologies. Nanotechnology holds great promise. For example, the MAO Group evaluates and designs oxide-based nanostructured photocatalysts for photodegradation and antibacterial wastewater treatment. They first understand the fundamental adsorption and reactive species generation kinetics and mechanisms, and develop quantitative relationships between activity and underlying mechanisms.

In another project, Mao and his students coat kale seeds with metal oxide nanoparticles and study the effects on plant growth.

Results demonstrate treating kale seeds with oxide nanoparticles at appropriate concentrations could proliferate growth and development of this healthy, fast–growing vegetable. These positive results have motivated further exploration in the agriculture and food industries.

These exemplary functional metal oxide nanomaterials explored by the MAO Group offer bright promises for producing innovative advances across multiple technologies, and substantially impacting our lives. The MAO research group has secured several million dollars in grants from agencies including the National Science Foundation, Air Force Office of Scientific Research, Defense Threat Reduction Agency, Defense Advanced Research Projects Agency, United States Department of Agriculture, American Chemical Society Petroleum Research Fund, and the Gates Foundation. For more detail about Mao and his research group visit: **https://science.iit.edu/people/faculty/yuanbing-mao**

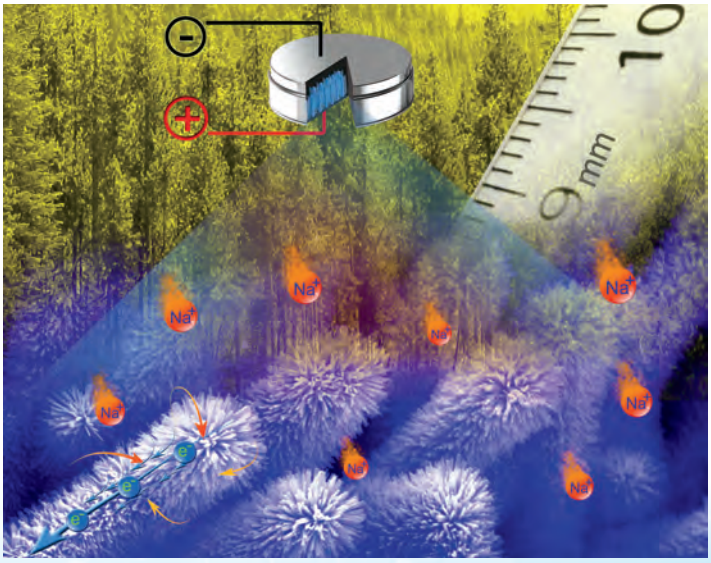


Figure 2: Schematic representation of three-dimensional metal oxide nanostructures for miniaturized energy storage devices with improved performance.

Robert "Bob" Filler (1984)

Robert Filler Will Be Remembered with Fondness

Reprinted from Illinois Tech Today: Robert "Bob" Filler, who, beginning in the 1950s, served as a professor of chemistry, chair of the Department of Chemistry, and dean of then-Lewis College of Sciences and Letters, passed away on January 8, 2019. He is remembered as being a passionate researcher and scholar who received numerous grants, published more than 180 papers, and advised many graduate students. Filler was an active member of the American Chemical Society from 1947, and in 1976 chaired the fluorine division. He lectured widely, serving as a visiting professor at universities in England, Israel, and Germany, as well as giving papers in Russia, Poland, and Japan. Filler also co-founded a research-and-development startup, working into his 90s. "After his retirement, he used to come to IIT for the love of science and to work with me," recalls Braja K. Mandal, longtime Illinois Tech professor of chemistry. "We had two decades of great research work—and more than 50 publications together."

From the Chicago Tribune obituary on January 10, 2019: "He was a lifelong sports fan, from the Brooklyn Dodgers to the Chicago White Sox. He loved to sing and dance with [wife] Miriam to classics like 'Let's Dance at the Make-Believe Ballroom.' When not traveling abroad, he loved showing his family the breadth and beauty of the United States, taking them to conferences and vacationing from coast to coast."

We recall Filler with a big smile on his face, belting out one of his favorite numbers in the department suite during his last visit to pick up his briefcase:

"New York, New York,
a helluva town!
The Bronx is up,
but the Battery's down
The people ride
in a hole in the groun'
New York, New York, it's a helluva town!"

—Excerpt from "New York, New York (What a Wonderful Town)" from *On the Town*

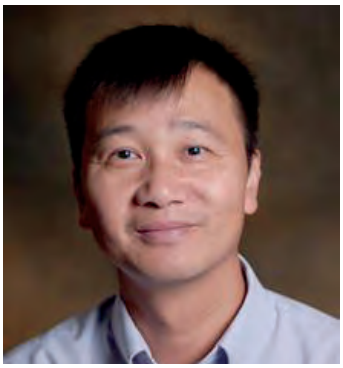
Chemistry Department 2019 Sigma Xi Award Recipients

The Illinois Tech chapter of Sigma Xi Scientific Research Honor Society held an event in The McCormick Tribune Campus Center on April 10, 2019. Two individuals from the Department of Chemistry received awards: The Student Award was given to Ph.D. candidate Elahe Moazzen for her research in the area of high-capacity alkaline batteries in the Segre Research Group; the

Junior Faculty Award was given to Associate Professor David Minh, who is actively pursuing research on implicit ligand theory and predicting molecular interactions to aid drug discovery.

Students in the professional analytical chemistry program (ACHM) visited campus for their final oral presentations on November 8. Shown here with Professor Yuanbing Mao, Chemistry Chair [third row, left]; Diep Nguyen, ACHM Program Director [first row, right]; and Gregory Webster, ACHM examiner from AbbVie Inc. [first row, left].

Two Faculty Promotions in 2018-19 Academic Year



Xiyun (Richard) Guan was promoted to full professor of chemistry. He was awarded tenure in spring 2015. Since arriving in 2013, Guan has maintained continuous funding and consistently publishes in high-quality journals. Guan is recognized as one of the worldwide leaders in nanopore sensing, and has been extremely successful in securing external funding from various agencies such as National Science Foundation and National Institutes of Health.

David Minh joined Illinois Institute of Technology in 2013, and has been promoted to associate professor with tenure in the Department of Chemistry. Minh is well respected in the community, and considered to be a rising star in the field of theoretical and computational chemistry. Recently he became associate director for the Center for Interdisciplinary Scientific Computation at Illinois Tech. He was one of three members of the academic community at Illinois Tech to receive the 2019 Halo Award. Minh will become a leader in the growing interdisciplinary area of scientific computation on the Illinois Tech campus, developing cross-departmental collaborations that will strengthen the research climate at the university. He was on sabbatical during the fall 2019 semester pursuing collaborations across the United States and overseas.

Mandal and Rogachev Receive WISER Awards

Professor Braja Mandal and Assistant Professor Andrey Rogachev received grant awards in 2019 from the the Wanger Institute for Sustainable Energy Research (WISER):

- "Theoretically Pre-Designed Supercapacitors with the Energy Density of Li-Ion Batteries," Rogachev with co-principal investigators Mandal and Carlo Segre, Duchossois Leadership Professor and professor of physics
- "Novel Polymer Electolytes to Prevent Dendrites in Lithium Metal Batteries," Mandal with co-P.I. Leon Shaw, Rowe Family Chair Professor in Sustainable Energy and professor of materials science and engineering

Minh Receives NSF Award for Collaborative Research Developing Software

David Minh, associate professor of chemistry, was awarded a $240,000 grant from the National Science Foundation (NSF/1905324) to pursue the development of statistical methods for studying molecular binding interactions. The title of the award is "CDS&E: Elucidating Binding using Bayesian Inference to Integrate Multiple Data Sources," in collaboration with Lulu Kang, associate professor of applied mathematics at Illinois Tech, and John Chodera from the Sloan-Kettering Institute for Cancer Research in New York.

Through integrating large amounts of data collected through the use of multiple analytical instruments and experimental protocols, the research team is developing new software to analyze chemical data in relation to molecule binding. Existing statistical methods and software do not fully integrate data from multiple sources to produce useful knowledge. The team's software constructs Bayesian networks that will be used to advance knowledge of cooperativity between binding sites.

Spring 2019 Student Awards

Chemistry Undergraduate Junior Award
Highest Achieving Junior
An Ling L. Engebretson (CHEM 3rd Year)

Chemistry Undergraduate Senior Award
Highest Achieving Senior
Joseph M. O'Shea (CHEM 4th Year)

Chemistry Teaching Assistant Award
Superior Service as a Teaching Assistant
Pearl Arora (CHEM Ph.D. candidate)

Other 2018–19 Student Awards

Damola Taye Shuaib, Ph.D. candidate in the Khan lab, was a recipient of the 2019 Graduate Student Research Award at ChemMatCARS. The National Science Foundation's ChemMatCARS is a National Synchrotron X-Ray User Facility located at the Advanced Photon Source at Argonne National Laboratory. Shuaib received a six-week summer stipend of $3,300.

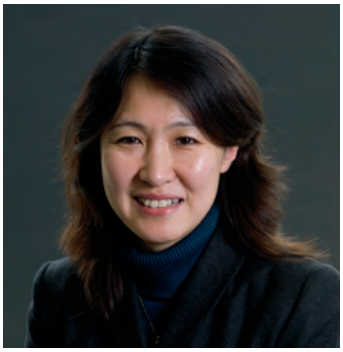
An Ling L. Engebretson (CHEM 3rd Year) received a 2019 Undergraduate Summer Research Stipend from the College of Science to work with Associate Professor David Minh.

Makaela Johnson, a junior at the Lindblom Math and Science Academy in Chicago, received a $2,500 American Chemical Society SEED award (Summer Experiences for the Economically Disadvantaged) as part of her research in Assistant Professor Jean-Luc Ayitou's lab last summer.

Professor Carlo Segre with Pearl Arora, Ph.D. candidate and winner of the 2018-19 TA Award

[left to right] An Ling Engebretson CHEM 3rd year; Dr. Ben Zion, advisor; Joseph O'Shea CHEM 4th year

Wang Receives NIH Award for Continuing Collaborations



Professor Rong Wang received an award for research titled "Matrix Mediated Electrical Stimulation of Fibroblast Cells for Restoring Biomechanics of Vaginal Wall Connective Tissues" from the National Institutes of Health (NIH/1R15HD096410-01A1). The three–year, $440,000 award will fund continuing collaborations with Dr. Svjetlana Lozo of the NorthShore Hospital and Dr. Margo Damaser of the Cleveland Clinic Lerner Research Institute. The research aims to transform the extracted fibroblast cells from pelvic organ prolapse (POP) patients *in vitro* by matrix mediated electrical stimulation. They also propose to examine the functionality of the transformed cells in remodeling the decellularized POP vaginal wall tissue matrix, and to evaluate the feasibility of transplanting the transformed fibroblasts to restore the biological function of vaginal wall connective tissues. Ideally, the group aims to create a simple localized cell injection therapy, making the procedure safe and affordable for patients.

Chemistry Forensics Field Trip

Associate Professor David Minh invited his spring 2019 CHEM 100 course students to visit the Illinois State Police Forensics Science Center facility for a tour on April 12. [From left] Shayna Casupang (Forensic CHEM 1st Year); Diana Csercse (BCHM 4th Year); Associate Professor of Chemistry David Minh; and Aaron Gregory (Forensic CHEM 2nd Year).

Professor Jean-Luc Ayitou was the Brown & Williamson Distinguished Guest Speaker at the University of Louisville on October 25. He presented his research on "Non-classical Aromatic Triplet Chromophores: Synthesis, Photophysics and Application in Light Harvesting & Energy Upconversion."

Congratulations to Our 2019-20 Kilpatrick Fellow

Youwen Zhang, Ph.D. candidate

Chemistry Poster Prize Winners

The poster prize winners from the interdepartmental picnic event Friday, August 16 were:

- **Makaela Johnson, high school research participant in the Ayitou lab**
- **Enya Mulroy (CHEM 3rd year)**
- **Dustin Woods (CHEM Ph.D. candidate)**

Degrees Conferred Academic Year 2018–19

Bachelor of Science in Chemistry
Grace Wischmeyer

Master of Chemistry in Analytical Chemistry
Bradley Berry, Kendall Jaderberg, Lindsay Rominger, Marsha Bures, Megan Frailey, James Lee, Shelby Lofthus, Taryn O'Connor, Teresa Paz, Mahmoud Awawda, Aura Goeppinger, Daniel Moseley

Master of Science in Analytical Chemistry
Brian Lane

Master of Materials Chemistry
Melody David, Anthony Lame, Lisa Wojnovich, Her Yang

Master of Chemistry
Dianchao Huang, Grace Wischmeyer

Master of Science in Chemistry
Hexi Zhang (thesis title: "Efficiency of Stratification for Ensemble Reduction Based on Docking Scores"); **Yuxin Ye** ("Solid-to-solid Photochemical Reaction of Covalent Organic Frameworks"); **Zhengyu Hu** ("Developing COFS to Study the Dimensionality of Energy Migration in Organic Solid")

Yuxin Ye (M.S. CHEM '19) commencement speaker

Ph.D. in Chemistry
Hamza Dunya, adviser Braja Mandal (dissertation title: "Nanostructured Sulfur Composite Cathodes for Lithium Sulfur Batteries"); **Siamak Shokri**, adviser Jean-Luc Ayitou ("Quinodization Reaction of Naphthalene Diimides to Afford Novel p-naphthoquinodimethane Light-Harvesting Chromophores: Aromaticity, Photophysics and Application for Photon Upconversion"); **Bing Xie**, adviser David Minh ("Implicit Ligand theory: Binding Free Energy Calculations Based on Multiple Rigid Receptor Snapshots"), **Zheng Yue**, adviser Braja Mandal ("Design, Synthesis and Characterization of Novel Materials to Construct High-Energy-Density Rechargeable Electrical Energy"); **Jingbai Li**, adviser Andrey Rogachev ("Chemistry of Buckybowl from Closed-Shell to Open-Shell").

2019 PhD Hooding Ceremony

Congratulations to our new PhDs!

ILLINOIS INSTITUTE OF TECHNOLOGY

Department of Chemistry
Robert A. Pritzker Science Center, Rm 136
3101 S. Dearborn Street
Chicago, IL 60616

Outstanding Chemistry Alum Received Honorary Doctor of Science for Contributions to the Development of a More Inclusive Society

Born in 1942 in Little Rock, Arkansas, **Gloria Ray Karlmark** (CHEM '65) is the granddaughter of a former slave and an Osage American Indian. Her father was educated by George Washington Carver and Booker T. Washington. Her mother held two university degrees and was the granddaughter of a plantation owner and a free black woman. Karlmark, at age 15, chose to attend Little Rock Central High School in 1957 and became known as one of the Little Rock Nine. The following year Arkansas's governor closed the public schools in Little Rock.

Karlmark and the other members of the Little Rock Nine have received a United States Congressional Gold Medal as well as numerous other awards, and a Little Rock Nine postage stamp and Desegregation in Education silver dollar were issued in their honor.

After receiving her bachelor´s degree, Karlmark worked as a school teacher, laboratory assistant, programmer, and mathematician until husband Krister Karlmark (M.S. DSGN '65)—who was once a professor at Illinois Tech's Institute of Design—accepted a job in Sweden. There she joined IBM's Nordic Laboratory and went on to learn Swedish at Stockholm University. After becoming a Swedish patent agent, she worked for IBM's International Patent Operations for 11 years. She then spent 13 years with various divisions of Philips in industrial documentation and as a patent specialist. Karlmark also co-founded and served as editor-in-chief of *Computers in Industry*, an international journal.

At the Illinois Tech May 2019 commencement, Gloria Ray Karlmark received an honorary doctor of science, *honoris causa*, for outstanding contributions to the development of a more inclusive society.