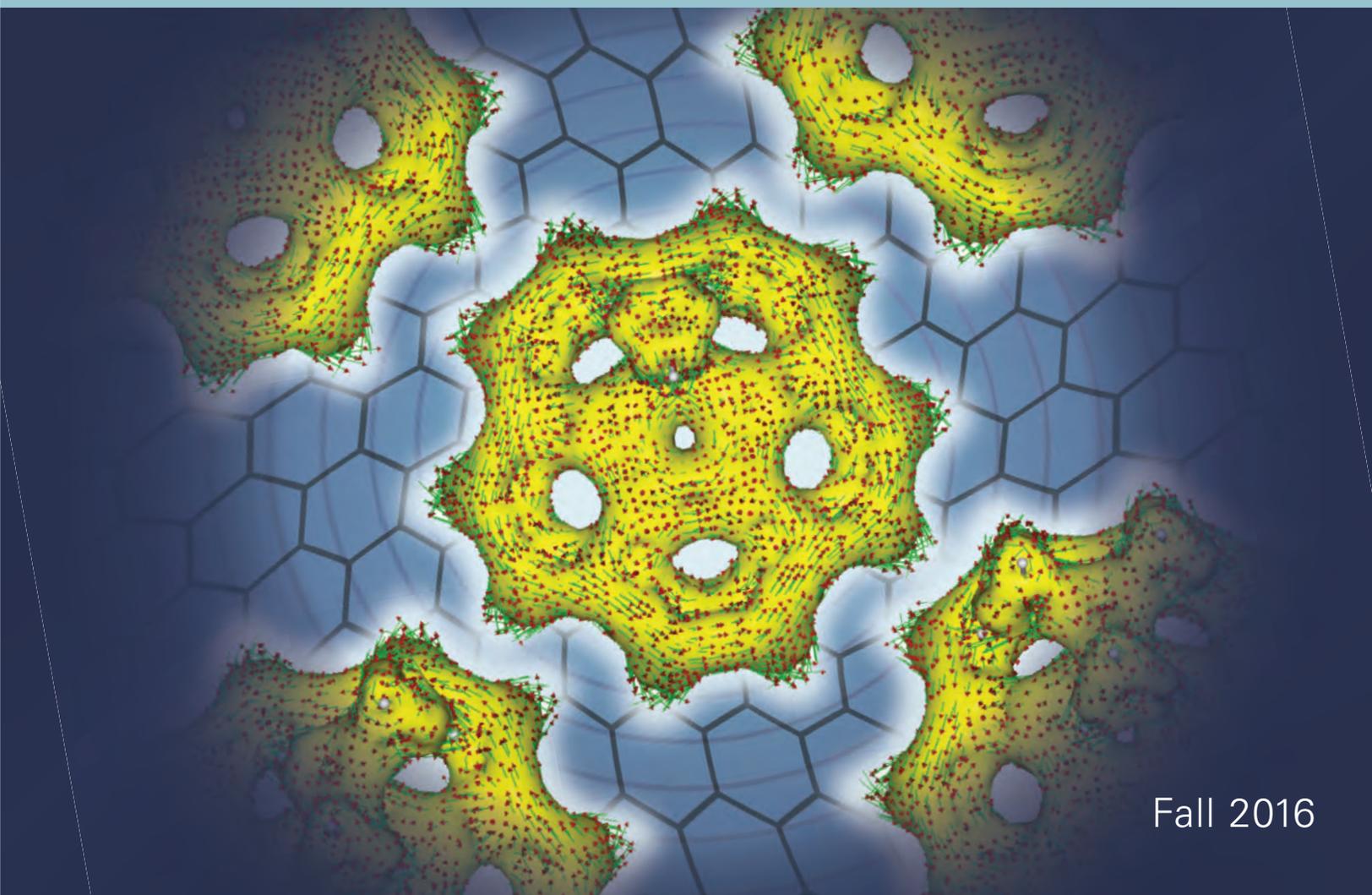
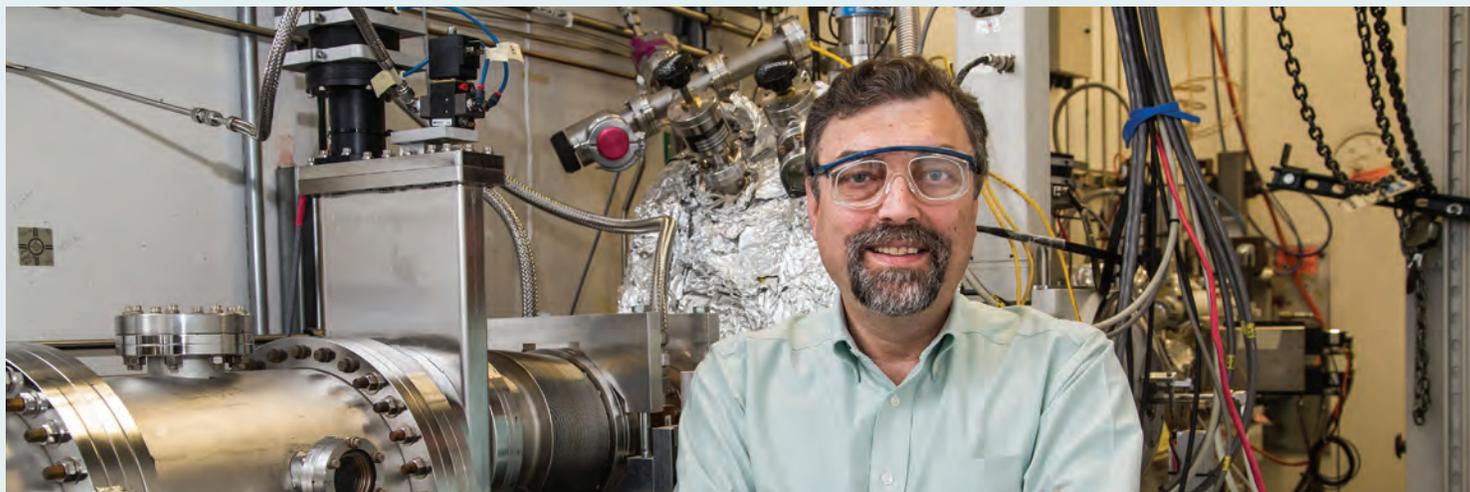


# CHEMISTRY ELEMENTS

A publication of the Department of Chemistry at Illinois Tech





## Letter from the Chair

As the new interim chair for chemistry, I am pleased to present our fourth issue of Chemistry Elements. After five years of service, Professor of Chemistry M. Ishaque Khan stepped down as interim chair last summer, and Dean Russell Betts appointed me to fill this position until fall 2018 as we initiate an external search for a new chairperson. In fact, I am returning to chairing chemistry, as I was executive chair of the department 25 years ago. We are grateful to Professor Khan for his leadership over the years in transitioning the division to a full, independent chemistry department. Among other things, he oversaw a complete curriculum revision of our undergraduate and graduate programs and led the department through a successful program review. Four new tenure-track faculty members were brought on board during his tenure, and the research area of computational chemistry was initiated through two of these hires. Khan helped increase the department's visibility through special events, and he focused our mission and vision for the future.

We have started our new academic year with many exciting developments to report.

Our professional master's program in analytical chemistry celebrates its 20th year! Former chemistry chairman Walter Eisenberg launched this program in 1996. We will be holding an event in March 2017 to celebrate this landmark occasion.

Our variety of co-terminal programs, which allow students to earn their bachelor of science and master of science degrees in as few as five years, is expanding. The Illinois Tech Board of Trustees approved three new co-terminal degrees involving chemistry: a B.S. in chemistry with an M.S. in chemistry, a B.S. in chemistry with an M.S. in biology for the health sciences, a B.S. in chemistry with an M.S. in sustainability management, and a B.S. in chemistry with an M.S. in chemical engineering.

Our undergraduate American Chemical Society chapter has continued to be active, and performed two chemistry shows last year, one of which coincided with Mole Day (the unofficial holiday celebrated among chemists on October 23) and the other a spring show.

This past year we awarded six more doctorate degrees as well as nine Master of Chemistry degrees in our full-time program. There were also nine graduates in our part-time professional master's degree programs.

We are happy to welcome our new Assistant Professor Anoklase Jean-Luc Ayitou, who comes to us from UCLA and works in the area of organic chemistry—specifically blending

organic synthesis and photochemical-photophysical sciences to target various applications in energy, materials, and sustainability. Among other faculty news, Adam Hock was promoted to associate professor with tenure. Hock has the largest research group in the chemistry department, focusing on catalysis and chemical structure and bonding. He continues his joint appointment with Argonne National Laboratory and provides highly collaborative research opportunities for students at Illinois Tech through this affiliation.

We have been watching with anticipation the second phase of the renovation of the Life Sciences building, which was renamed the Robert A. Pritzker Science Center on September 21; we look forward to using this new space and watching students enjoy it, as we have seen with our now very popular west lobby. Additionally, the third floor of the Tech South building became the new home for assistant professors Andrey Rogachev's and David Minh's research groups, whose growth required larger spaces.

Lastly, alumnus Ted Erikson (CHE '52, M.S. CHEM '59) was recognized at this past year's Alumni Awards luncheon, where he received the John J. Schommer Honor I Award for his career in professional swimming.

On behalf of the faculty and students, I want to extend a hearty thanks for your continued support. We have seen donations come in from chemistry alumni around the country, and this has made a big difference in helping to strengthen our department programs.

### Carlo Segre

*Interim Chair, Department of Chemistry  
Duchossois Leadership Professor  
Professor of Physics*

**COVER IMAGE:**  
magnetic vector  
field of man-  
made molecule,  
corannulene.





◀ Analytical Chemistry Program Director **Diep Nguyen** with graduate **Joy Gravitt**.

## Celebrating the Nation's First Professional Science Master's Program

Professional education for scientists? What a concept! Yet this year, Illinois Tech is celebrating the 20th anniversary of its first professional science master's degree, and incidentally, the first of its kind in the nation: the master's in analytical chemistry.

This degree provides an alternative to an academic career—an alternative leading to a fruitful career in business, industry, the military, or government. Twenty years from its inception, scientists can now choose from over 350 professional science degrees nationwide.

In 1996 Professor Walt Eisenberg, former chair of chemistry at Illinois Tech, understood the need for well-trained chemists in industry. He saw entry-level chemists with bachelor's degrees and senior research Ph.D.s, but a dearth of chemists with the advanced training and the business skills needed in industry. Eisenberg thus created a curriculum that included project management and communication as well as advanced analytical chemistry courses.

When Eisenberg designed the program for working chemists who needed to further their education, he realized that they would not be able to quit their jobs to go back to school and that taking night classes might be too burdensome on their home lives. So he offered the program through closed circuit TV at 40 satellite locations in the Chicago area. Two years later the program went online and the rest is history. Illinois Tech has since awarded more than 160 Master of Analytical Chemistry degrees and has a steady enrollment of about 50 students. The students and graduates work in a variety of sectors including cosmetics, paints and coatings, semiconductors, food packaging and processing, pharmaceuticals, forensics, and health care.

For programs to last over the long term they must be adaptable. Industry Professor of Chemistry Diep Nguyen, who took over the program in 2006, has been in tune with industry's needs and has bolstered the program's reputation while maintaining its relevance and rigor. Since the students have on-the-job laboratory experience at their workplace and therefore do not require laboratory courses, more attention can be paid to broaden the students' education. Illinois Tech offers courses in molecular spectroscopy, atomic spectroscopy, the fundamentals of separation science, physical methods of characterization, and statistics. The program culminates in a final capstone project, which the students present to a panel of examiners.



### Come Celebrate with Us!

In March 2017 the chemistry department will honor Walt Eisenberg and 20 years of analytical chemistry at Illinois Tech. For more details or to get involved, contact Director Diep Nguyen 312.567.8924 or [nguyen@iit.edu](mailto:nguyen@iit.edu).

For more information about the master's degree in analytical chemistry and associated certificate programs, visit [science.iit.edu/chemistry](http://science.iit.edu/chemistry).

## New Faculty Appointment

Illinois Tech welcomes **Anoklase Jean-Luc Ayitou** as assistant professor in organic chemistry. Ayitou's research involves blending conventional synthetic organic chemistry and established concepts and techniques in photophysics and photochemistry to devise alternatives and complementary approaches for energy applications, organic materials, and sustainable chemical synthesis. His group's primary focus is energy transfer in organic solids. Specifically, Ayitou's research group will be investigating the diffusion and annihilation of excitons that originate from organic chromophores in the solid state. Additionally, his group envisions making use of the organic chromophores of their interest to devise electronic materials/devices and to engineer novel 2-D frameworks for various applications such as patterning, drug delivery, and stimuli-responsive graphene-like sheets. Another area of interest is synthetic organic photochemistry and photocatalysis with an emphasis on green and sustainable reaction conditions.

After completing an associate's degree in physics and chemistry from the Université de Lomé in Togo, Africa, Ayitou earned his B.S. degree and Ph.D. at North Dakota State University. He then continued his research training as a UNCF-Merck Postdoctoral Fellow and University of California President's Postdoctoral Fellow at the University of California, Los Angeles. At UCLA, he investigated Brownian Rotatory Dynamics in Photoresponsive Crystalline Molecular Rotors under UV and Vis irradiations. He used cutting-edge solid-state nuclear magnetic resonance techniques to probe Brownian rotatory motions in crystalline solids, and he also employed pump-probe spectroscopy techniques to rationalize the mechanisms and kinetics of light-initiated processes in crystalline organic chromophores.





## Powder Crystallography of Real Materials

James Kaduk, research professor of chemistry at Illinois Tech since 2010, is an expert in crystallographic analysis and problem solving, and a great resource for faculty and students at Illinois Tech.

Thanks to a donation from Kaduk, the Center for Synchrotron Radiation Research and Instrumentation (CSRRI) was able to purchase an X-ray powder diffractometer, which has been used by many graduate and undergraduate students across the Illinois Tech campus. He has also contributed to the recently completed acquisition of a single-crystal diffractometer, which will also be housed in the CSRRI.

Kaduk holds a Ph.D. in inorganic chemistry from Northwestern University. He is owner and president of Poly Crystallography, Inc., which provides crystallographic consulting and problem-solving services, mainly using powder diffraction techniques. Previously, Kaduk worked for Amoco Chemicals in catalysis research and development and then INEOS (formerly BP Chemicals). He has published nearly 200 research papers.

He is a past chair and current treasurer of the International Centre for Diffraction Data (ICDD), the organization that produces the Powder Diffraction File, a database containing the patterns of more than 800,000 pure compounds. Kaduk has also served as chair of the U.S. National Committee for Crystallography.

As part of these affiliations with crystallography, Kaduk travels quite a bit, teaching short courses and workshops, and “getting IIT’s name out around the world.” In March 2016 he traveled to India for a meeting of the Program Committee for the International Union of Crystallography and has visited Chester, England, several times for editorial meetings,

as he is one of the three main editors of the forthcoming Volume H of the International Tables for Crystallography on powder diffraction.

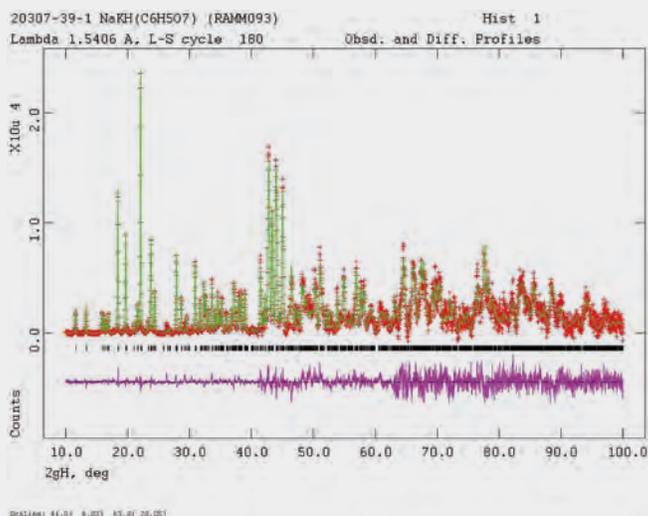
In his research, Kaduk has been focusing on several areas: citrate salts (commonly encountered as calcium supplements and Viagra, for example), catalysts, pharmaceuticals, long skinny molecules such as aliphatic carboxylic acids and metal soaps (which are used as polymer additives), and hydrogen bonding (important contributors to holding crystal structures—and us—together). Through curiosity-driven synthesis of alkali metal hydrogen citrates, Kaduk has recently encountered some of the shortest and strongest charge-assisted O-H...O hydrogen bonds.

The crystal structure provides the fundamental basis for understanding the physical properties of a solid-state material, and most crystal structures are determined using single crystal methods. Until now, we have not had this capability at Illinois Tech; but as of September 2016, we now have a benchtop single crystal diffractometer as shared equipment managed by the CSRRI and available to the entire campus.

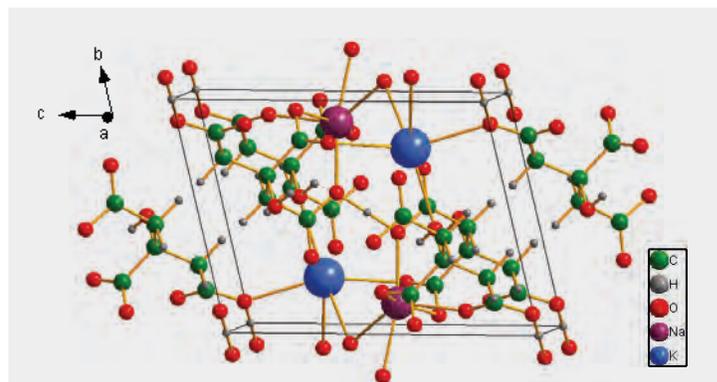
However, many real materials are not obtainable as single crystals. Fortunately, improvements in data quality, algorithms, and computer power have made it increasingly possible to solve crystal structures using powder diffraction data. Techniques used include direct methods, real space geometry optimization, Monte Carlo simulated annealing, charge flipping, “stealth and guile,” and working by analogy. Determination of a crystal structure from scratch can be straightforward, but more often it is a true research project.

A good rule is that a single crystal will yield more accurate and more precise results, and you should use it. But if you can’t grow the crystal, you can still solve the structure using a powder X-ray diffractometer.

Most real materials are composed of large numbers of very small crystallites (polycrystalline) and are ground into powders for analysis. X-ray diffraction (XRD) can be used to characterize any solid crystalline material. X-ray powder diffraction is one of the most versatile analytical techniques, able to provide not only qualitative and quantitative phase analysis, but also details of atomic, molecular, and crystalline structure as well as information on microstructural properties such as crystallite size, strain, and texture. Systems commonly studied include catalysts, corrosion and process deposits, metals and alloys, minerals, ceramics, cements, small organic molecules, pharmaceuticals, coordination complexes, polymers, and foodstuffs. The range of



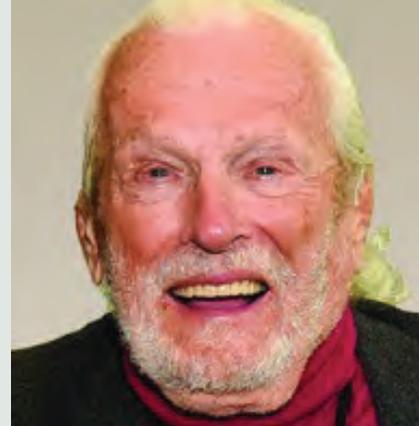
Rietveld plot for the refinement of  $\text{NaKHC}_6\text{H}_5\text{O}_7$ . The red crosses represent the observed data points, and the green line is the calculated pattern. The magenta curve is the difference pattern, plotted at the same scale as the other patterns. The vertical scale has been multiplied by a factor of 6 for  $2\theta > 41.0^\circ$ , and by a factor of 20 for  $2\theta > 63.0^\circ$ . The row of black tick marks indicates the reflection positions for the phase.



Crystal structure of sodium potassium hydrogen citrate, viewed approximately down the a-axis.

# Chemistry Alumnus Ted Erikson Honored at Luncheon

Ted A. Erikson (CHE '52, M.S. CHEM '59) was the 2016 John J. Schommer Honor I Award recipient at the Alumni Awards luncheon in April 2016, where he was recognized for his career in professional swimming. Among other accomplishments, in 1965, Erikson set the world record for the fastest round-trip swim of the English Channel (England-France-England)!



*continued from page 4*

applications is very wide. Analysis can be carried out not only at ambient conditions, but also *in situ* at high or low temperatures and in controlled atmospheres. XRD is one of the very few techniques capable of providing structural information at real process conditions. Solid samples, such as metals and polymers, are also easily analyzed.

Generally, ~1 gram of solid is convenient to analyze, but much smaller quantities can be used if necessary. If the sample can be seen visually, it is generally possible to obtain diffraction data. Most academic crystallography is performed on single crystals, generally 50–300  $\mu\text{m}$  in size (though smaller crystals can also be used).

When a beam of X-rays illuminates a single crystal, many “spots” are generated. The positions of the spots are determined by the size and shape of the unit cell and the symmetry. The intensities of the spots are determined by the arrangement of the atoms within the crystal. After measuring the intensities of all of the diffraction spots (reflections), it is generally possible to determine the positions of the atoms in the unit cell (the structure) in a straightforward manner. Sometimes, however, the sample is more complex (twinning, aperiodic structure, diffuse scattering), and the structural analysis becomes a challenge for even the most skilled crystallographers.

Kaduk uses several databases as reference for well-characterized compounds (where the identity is known). He notes that a large number of pharmaceutical crystal structures are unpublished. For example, folic acid, a vitamin supplement frequently used by pregnant women, was unpublished until last year. In practice, the experimental powder pattern is searched against the Powder Diffraction File database.

The ICDD, Illinois Tech, and the Advanced Photon Source at Argonne National Laboratory have established a project to generate high-quality reference powder data for pharmaceutical compounds and to determine the crystal structures when they are not available.

Employing sophisticated data analysis, Kaduk generally uses the Rietveld method. In Rietveld analysis, all of the structural information and diffraction physics we know is used to carry out a least-squares modeling of the raw diffraction data. This analysis extracts the maximum information from the data, and thus provides the most value per analysis. Crystallographic results are often complemented by density functional quantum calculations. Density functional calculations are essential to complete the crystal structures and understand the bonding, particularly the hydrogen bonding. Combining crystallography and quantum mechanics achieves an understanding of not just where the atoms are, but why they are there. The interplay between experiment and theory is critical for a complete understanding of the structures.

Kaduk has contributed more than 700 patterns to the Powder Diffraction File and has written 20 papers in the last year and a half. He believes that when it comes to crystal structures, “You know it will be important, but you just never know when.”

## Our Alumni— Where are They Now?



◀ **John Clark** (CHEM '15) was our 2016 Commencement speaker. Following graduation, Clark began working at Procter & Gamble in Phoenix.



◀ **Leonard Edwards** (M.A.S. CHEM '16) is now working as an environmental specialist at the Metropolitan Water Reclamation District of Greater Chicago.



▲ Pictured here at the 2016 Ph.D. hooding ceremony are [left to right] **Xinyi Mei, Shuo Zhou, Professor Rong Wang, Wen Li, and Lili Kang.**

**Bo Hu** (Ph.D. CHEM '15) is a postdoc at Georgia Institute of Technology, where he is working on the design and synthesis of new catalysts for membrane reactor applications and a preparation of new types of polymers for CO<sub>2</sub> capture.

**Matt Weimer** (Ph.D. CHEM '16) is currently a postdoc at Argonne National Laboratory in the Chemical and Sciences Division, where he is using hard X-rays, powder diffraction and pair-distribution function, and atomic force microscopy to understand deactivation mechanisms in battery anodes.

**Shuo Zhou** (Ph.D. CHEM '16) is an assistant research scientist at the Chongqing Institute of Green and Intelligent Technology, which is part of the Chinese Academy of Sciences.

## Faculty News

**Adam Hock** was promoted to associate professor with tenure beginning fall semester 2016.

Assistant Professor **David Minh** gave an invited talk entitled "Emerging Methods for Second-Stage Virtual Screening" for the Free Energy Methods in Drug Design Conference at Vertex Pharmaceuticals in Boston in May 2016.

Industry Professor **Diep Nguyen** presented a talk, "Next Step in Your Education: A Professional Master's Degree in Chemistry," at the Biennial Conference on Chemical Education, held in Greeley, Colorado, in August 2016.

Assistant Professor **Andrey Rogachev** had his article "Stability of functionalized corannulene cations [R-C<sub>20</sub>H<sub>10</sub>]<sup>+</sup>: An influence of the nature of R-Group" featured on the cover of the *Journal of Computational Chemistry*, Vol. 37, Issue 25, September 2016 [see cover image]. Rogachev received funding in 2016 for his project "Programmable Molecular Transformations" from ChemRing Ordnance Inc./DOD-DOTC/DARPA. He gave an invited talk on "Sumanene as New Material for Supramolecular Aggregates" at the CERM 2016 American Chemical Society Central-East Regional Meeting, in Covington, Kentucky, on May 18–21 and another invited talk on "Buckybowls: A Theoretical Point of View" at Roosevelt University in Chicago on March 28.

Professor **Rong Wang** received funding through the Pritzker Institute of Biomedical Science and Engineering, as a collaborator with Eric Brey, Duchossois Leadership Professor and professor of biomedical engineering.

Chemistry Lecturer **Ben Zion** was appointed senior lecturer and associate chair beginning fall semester 2016.

Chemistry Laboratory and Course Coordinator **Zabel Panosyan** was recognized for her years of service to the department. She is pictured with President Alan W. Cramb at the 2015 Staff Service Awards event. ▼



## Student News

### 2015–16 Degree Recipients

Three students received a **Bachelor of Science in Chemistry** degree last year: Khadijah Pullen, Maximilian Vitas, and John Clark.

The following students received master's degrees in chemistry:

**Master of Chemistry:** Leonard Edwards, Shengnan Jin, Zehui Li, Xiaojian Lian, James Rice, Yuwei Xiao, Yunjie Xu, Yu-ting Yu, and Jingyang Zhang

**Master of Chemistry in Analytical Chemistry:** Danielle Cornett, Joy Gravitt, Syed Jawaaid, Heather Jones, Michelle Menze, Noah Morgan, Brian Roemer, Laura Twentier

**Master of Chemistry in Materials Chemistry:** Andrew Cohen

Six new **Ph.D. degrees** were awarded in 2015–16. Recipients are (with dissertation titles):

**Bo Hu**—"From Exploration to Rational Design of Single-Site Heterogeneous Catalysts for Selective Propane Dehydrogenation"

**Lili Kang**—"Synthesis and Post-Synthetic Modification of Tetrazine-Based Organic Frameworks"

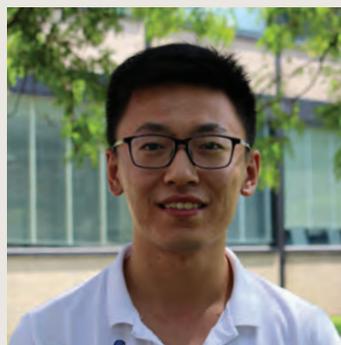
**Wen Li**—"Unidirectionally Aligned Collagen/Collagen Composite Fibrils and Their Modulation of Cell Behaviors"

**Xinyi Mei**—"New Solid and Liquid Electrolytes for Lithium Rechargeable Batteries"

**Matt Weimer**—"Understanding Reaction Mechanisms and Controlling Reactive Surface Species during Atomic Layer Deposition of Metal Chalcogenides"

**Shuo Zhou**—"Nanopore Stochastic Sensing of Biomarkers in Human Disease"

## Congratulations to Our 2016–17 Fellows!

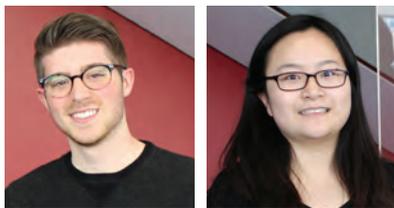


▲ Ph.D. candidate **Xiang Lu**, 2016–17 Tang Fellow



▲ Ph.D. candidate **Jingbai Li**, 2016–17 Kilpatrick Fellow

## Spring 2016 Student Award Recipients



◀ **Undergraduate** student **Nicholas Politis** (CHEM 4th year) was awarded the 2015–16 Junior Award last spring, and **Dan Yin** (CHEM 5th year) was awarded the 2015–16 Senior Award.



◀ **Graduate** students **Zirui Zhang** and **Jose Orozco** were jointly awarded the 2015–16 Teaching Assistant Award.

◀ Zirui Zhang [right] with Lecturer Courtney Sobers



◀ Jose Orozco [center] with advisor, Professor M. Ishaque Khan [left], and Lecturer Ben Zion [right]

Four **Ph.D. candidates** were given Fanta Award funding over the past year to attend conferences:

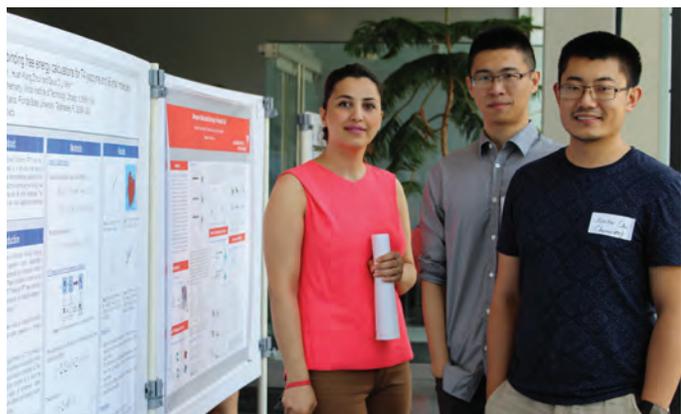
**Naiwei Chi** attended PITTCON in Atlanta in March 2016.

**Jingbai Li** attended the August 2016 ACS meeting in Philadelphia, presenting the talk "Aromatic Stabilization of Functionalized Corannulene Cations."

**Elahe Moazzen** attended the 65th Denver Conference on Applications of X-ray Analysis, held in Rosemont, Illinois, in August 2016. Her talk was titled "Synthesis of  $\text{MnO}_2$  Nanomaterials with Fine Control of Morphology and Crystalline Phase Composition." Moazzen also presented at the AVS Prairie Symposium in Science and Technology of Materials, Interfaces, and Processing, held at Illinois Tech in September 2016.

**He Zhang** presented on "Organometallic Chemistry Approach to Crystalline Tungsten Disulfide" at the August 2016 ACS meeting in Philadelphia. He also gave a talk entitled "XAFS Observation of Nucleation Mechanism in Deposition of  $\text{WS}_2$ " at the August 2016 Denver Conference in Rosemont.

Chemistry graduate students **Golbag Mohammadiroozbahani**, **Xiaohan Chen**, and **Naiwei Chi** attended the annual poster session picnic on August 18. Chemistry joined the biology and physics departments for this event, where nearly 50 research posters were presented. ▼



## Spring 2016 Chemistry Show



◀ **Nicholas Politis** (CHEM 4th year) performs the "chemical traffic light demo," in which shaking the solution introduces oxygen, causing a color change from yellow to green to red to yellow.



◀ **Andrew Shahidehpour** (CHEM 2nd year) holds up a supersaturated solution to which he added a crystal of sodium acetate, initiating the blooming phenomenon while releasing heat in an exothermic reaction.



◀ **Ismael Sanchez** (CHEM 2nd year) demonstrates the fluorescent properties of fluorescein, the original dye used to turn the Chicago River green, while Andrew Shahidehpour looks on. The dye is dark when in a concentrated solution but glows a bright green when diluted.



◀ **Abdallah Hasan** (CHEM 1st year) brings a new twist to "April showers bring May flowers" by turning a muddy yellow solution into beautiful golden crystals in a simple double replacement reaction.



◀ **Grace Wischmeyer** (CHEM 4th year) demonstrates a combination of two clear liquids that turn into a solution that glows a very bright blue. This solution contains luminol, the chemical used to detect blood at crime scenes.

The **Illinois Tech ACS Club** toured Argonne National Laboratory on September 10. **Courtney Sobers**, lecturer of chemistry and faculty advisor, led the tour. ▼



Department of Chemistry  
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Chicago, IL 60616

## Life Sciences Building Becomes the Robert A. Pritzker Science Center

Illinois Tech trustees, donors, faculty, staff, and students gathered on September 21 for the Robert A. Pritzker Science Center dedication ceremony. A biographical photographic tribute was installed in the entrance of the building to highlight the life of the late Robert A. Pritzker (IE '46). ►

*[Left to right]* President Alan W. Cramb, President Emeritus Lew Collens, Life Trustee Jamie Cowie, Col. Jennifer N. Pritzker, Andrew Pritzker, Chairman of the Board of Trustees Bud Wendorf (ME '71), Trustee Mayari Pritzker (Ph.D. PSYC '01), College of Science Dean Russell Betts, former chairman of the board and University Regent John Rowe ▼

