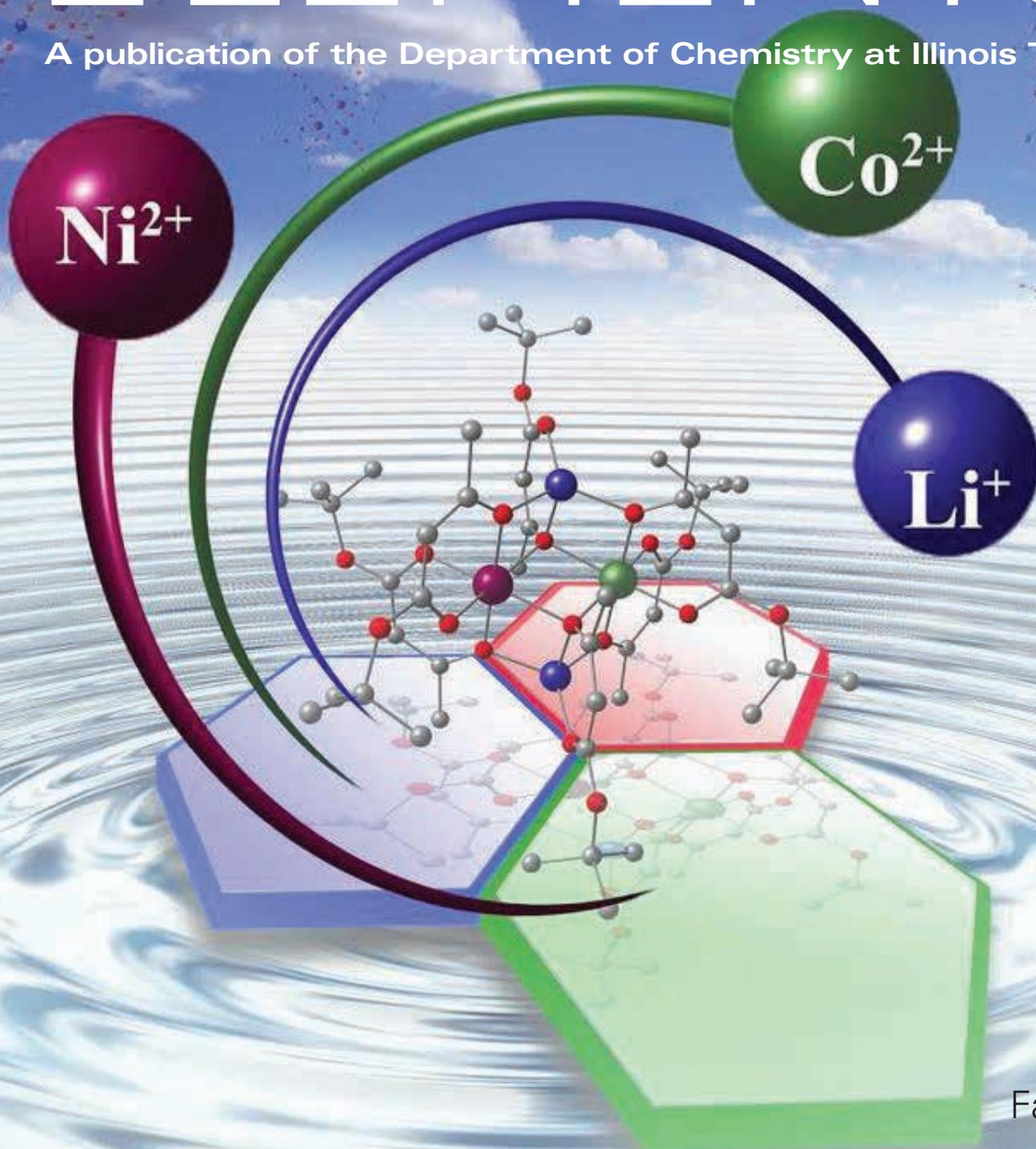
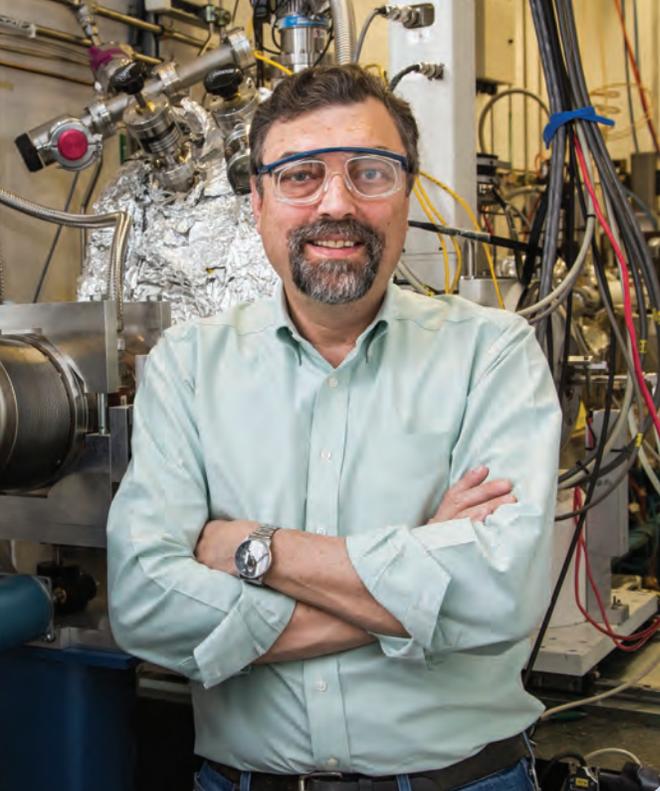


CHEMISTRY ELEMENTS

A publication of the Department of Chemistry at Illinois Tech





Welcome to the sixth annual issue of *Chemistry Elements*. You may be surprised to hear from me once again; however, we have continued our department chair search into the 2018–19 academic year. Unfortunately, we were unable to complete the search in spring of 2018, and I was asked by the chemistry faculty to continue as the interim chair for a third year. We are very optimistic that the search will conclude successfully in the spring of 2019 and that the new chair will start in the summer of 2019 with fresh ideas for strategic planning and growth.

Following are a few updates:

I am happy to report that we now fully support all of our Ph.D. students and our undergraduate enrollment is up. Additionally, if you have not heard, Illinois Tech's overall rating in *U.S. News & World Report* climbed to 96 among national universities.

Our first co-terminal students graduated: Congratulations to Yinan Wang, who graduated cum laude, and Nick Politis, who graduated summa cum laude.

Letter from the Chair

Recognizing that the Master of Science is the more preferred degree in the graduate student population, the Illinois Institute of Technology Board of Trustees approved the new Master of Science in Analytical Chemistry (which replaces the Master of Chemistry degree).

In the research realm, we acquired two new instruments for the department: a Spotlight FT-IR (Fourier-transform infrared spectroscopy) microscope in the Jean-Luc Ayitou laboratory, and a Leica DMI8 microscope system, which will be used by the biology-focused faculty in the department. Our Raman microscope is now fully functional.

Around the time of the last newsletter printing, we learned that Ayitou had won the prestigious Faculty Early Career Development Award from the National Science Foundation, which provides \$650,000 for five years. He is the very first chemistry professor at IIT to receive this career-changing recognition and plans to use the funds to devise next-generation organic photonic materials. He has also started a science outreach program for young students in Chicago. Adam Hock received a Joint University Microelectronics Program (JUMP) grant from the Semiconductor Research Corporation—with the University of Notre Dame as lead organization. The project was proposed over five years to develop new chemistry

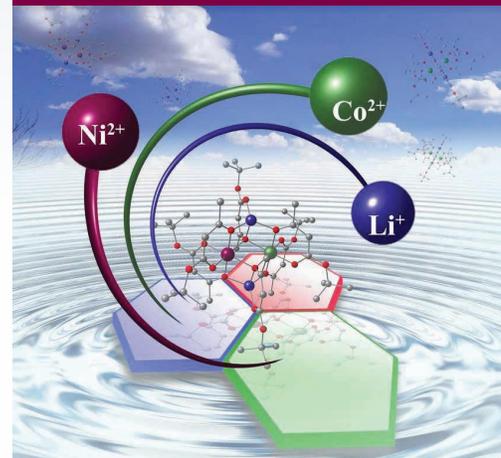
and precursors for the fabrication of semiconductor devices. David Minh also received a large award (with Oscar Juarez in Biology) from the National Institutes of Health entitled "Entropy for End-Point and FFT-Based Binding Free Energy Calculations."

Keep in touch—we would really enjoy hearing from you—and again, we hope you will visit the department if you are in the area. Wishing you a happy and healthy 2019.

Carlo Segre

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

COVER IMAGE: Image created by Jingbai Li, Ph.D. candidate in the Rogachev research group, depicting a genuine heterometallic molecule, the subject of which was published in *Chem. Sci.*, 2018, 9, 4736.





Jean-Luc Ayitou had an eventful summer attending the Reaction Mechanisms Conference 2018 in Vancouver, Canada, and the 27th IUPAC International Symposium on Photochemistry, July 8–13 in Dublin, Ireland.

First Illinois Tech Chemistry Professor to Win NSF CAREER Award

Jean-Luc Ayitou, assistant professor of chemistry, has won the Faculty Early Career Development (CAREER) Award from the National Science Foundation, Division of Chemistry: Chemical Structure, Dynamics and Mechanisms. The award (NSF/1753012), totaling \$650,000 for five years, is for his research on novel polycyclic chromophores that exhibit anti-aromaticity. Anti-aromatic compounds are thought to be far less stable than their aromatic counterparts, but these molecular systems possess attractive photophysical properties that are highly sought in photonic materials science. Ayitou is proposing to devise new synthetic strategies to prepare these novel organic chromophores and their corresponding light-harvesting dyads, which can be employed for photon upconversion. Photon upconversion is an elegant and sustainable solar energy management approach that can help maximize the efficiency of current photovoltaic devices or solar cells that can absorb light and produce electricity.

Ayitou and his team will use the tools of synthetic organic chemistry, computational modeling, advanced spectroscopy, and X-ray diffraction crystallography to accomplish the proposed project, which presents a mosaic of scientific techniques. They hope to exploit the outstanding photophysical properties

of the proposed organic light-harvesting systems to devise next-generation organic photonic materials. These novel materials can be further derivatized to engineer not only high-efficiency photovoltaic devices but also materials for biological imaging, among other applications.

As part of this project, Ayitou has started an outreach program in an effort to promote diversity and a better understanding of socio-cultural relevance of the chemical sciences and other STEM disciplines. The program, VISCUS (Vivifying Scientific Curiosity for Underrepresented Undergraduate Students), will allow him to mentor and provide training for students who will participate in the proposed research. Additional educational components of the program include outreach activities that promote STEM education. The students involved in VISCUS are expected to serve as ambassadors for STEM research in their respective communities.

The NSF CAREER Awards honor early career-development activities of teacher-scholars who most effectively integrate research and education within the context of the mission of their organization. Such activities should build a firm foundation for a lifetime of integrated contributions to research and education.

Assistant Professor Jean-Luc Ayitou hosted the first Illinois Tech science café for the community on June 23 entitled "STEAMing (Science, Technology, Engineering, Art, and Mathematics) Dialogue." Ayitou developed the new science cafés with Alicia Bunton, director of community affairs, to inspire future scientists in the community. He also hosted a Family Fun Day with the undergraduate chemistry club on September 15. Family Fun Day included an event to explore chemistry with a demonstration performed by the club members.





Minh and Juarez Receive NIH Grant for Predicting Molecular Interactions to Aid Drug Discovery

The research groups of David Minh, assistant professor of chemistry, and Oscar Juarez, assistant professor of biology, have received an award from the National Institutes of Health (NIH/1R01GM127712-01A1) entitled "Entropy for End-Point and FFT-Based Binding Free Energy Calculations." The award is for \$331,629 in the first year and is anticipated to total \$1.3 million over four years.

The main objective of this project is to develop better ways to account for entropy in two popular techniques for studying molecular interactions: "end-point" simulations of the bound complexes and their unbound counterparts, and molecular docking based on the Fast Fourier Transform (FFT), a mathematical operation for decomposing a function into representative frequencies. Specifically, new ways to analyze calculation results will be derived, implemented, assessed, and optimized. Additionally, the methods will be combined with enhanced sampling techniques.

Minh will also work with Juarez to assess the methods in a drug-discovery project. They will use established methods and these new methods to virtually screen a chemical library against a pair of structurally similar bacterial metabolic enzymes; one enzyme is relevant to active and the other to dormant bacteria. Compounds predicted to selectively bind the bacterial (opposed to human) enzymes will be experimentally

tested in biochemical assays. The researchers anticipate that their improved methods will be significantly more accurate than established approaches. On November 28, Minh received the 2018–19 Junior Research Award from the College of Science.



2017–18 Junior Research Faculty Award Given to Andrey Rogachev

Andrey Rogachev, assistant professor of chemistry, was honored for excellence in research in the junior faculty category of the College of Science. Rogachev's group has performed breakthrough buckyball research, discovered an efficient tool for fine-tuning magnetic coupling between delocalized radicals, and more. He had eight publications in 2018, six publications in 2017, and eight in 2016, and his research has appeared on a number of journal covers. Rogachev, who received his Ph.D. from Moscow State University, previously worked as a postdoc with Nobel Laureate Roald Hoffmann at Cornell University.

Segre and Timofeeva Publish Three New Papers on Battery Research

Illinois Tech researchers recently published three new papers that study the structural basis for improved battery electrode performance and suggest that higher capacities are possible with engineered materials. The researchers are Carlo Segre, interim chair of the Department of Chemistry and Duchossois Leadership Professor of Physics; Elena Timofeeva, research associate professor of chemistry;

and chemistry and physics Ph.D. candidates Elahe Moazzen, Shankar Aryal, and Yujia Ding.

The first paper, "Role of Crystal Lattice Templating and Galvanic Coupling in Enhanced Reversible Capacity of Ni(OH)₂/Co(OH)₂Core/Shell Battery Cathode," was published in *Electrochimica Acta*. The study explored novel core/shell nanoscale architectures for nickel hydroxide electrodes for aqueous rechargeable batteries. The findings of this study showed that a cobalt hydroxide additive, typically considered as inactive material, can also be part of a reversible charge and discharge reaction, adding to the material's capacity. The reversibility of the cobalt hydroxide redox reaction is dependent on the Co(OH)₂ shell thickness around the Ni(OH)₂ core nanoparticles, with the optimal thickness leading to a more complete utilization of the nickel hydroxide and enhanced performance.

The next paper, "Structural Studies of Capacity Activation and Reduced Voltage Fading in Li-Rich, Mn-Ni-Fe Composite Oxide Cathode," was published in the *Journal of The Electrochemical Society*. Lithium-ion batteries have the advantage of high cell voltage and high energy density, which make them first-choice solutions for portable electronic devices, electric vehicles, and stationary energy storage. Only a few types of lithium-ion battery cathode materials are currently used

in commercial cells, including cobalt-based layered oxides, iron-based olivine phosphates, and manganese-based spinel oxides. As cobalt is expensive and toxic, attempts have been made to replace it with cheaper and more environmentally friendly iron. This study investigates the mechanisms behind the reversible capacity and reduced voltage-fading mechanisms of nanoscale cobalt-free, lithium- and manganese-rich cathodes, specifically the complementary role played by the intimate mixing of two distinct structures that are present in these compounds.

The third paper, published in *Advanced Energy Materials*, is "In Situ EXAFS-Derived Mechanism of Highly Reversible Tin Phosphide/Graphite Composite Anode for Li-Ion Batteries." This study examines the reversibility of an anode material for lithium-ion batteries. Tin phosphide is a conversion-type material with high theoretical capacity but poor cycling performance. However, this study demonstrated that higher reversibility can be achieved through formation of a nanocomposite with graphite. Using the advanced X-ray characterization techniques available through Illinois Tech's Center for Synchrotron Radiation Research and Instrumentation, this paper reveals the detailed structural mechanisms contributing to the high reversibility of nanocomposite and explains



Segre research group [Left to right]: Elena Timofeeva, research associate professor of chemistry; Ning Su, Master of Science candidate in physics; Yujia Ding, Ph.D. candidate in physics; Kamil Kucuk, Ph.D. candidate in physics; Elahe Moazzen, Ph.D. candidate in chemistry; Huanbo Sun, Master of Science candidate in physics; Ryan Arnold, co-terminal Master of Science candidate in physics; and Professor Carlo Segre

the fading mechanisms in regular tin phosphide. This research indicates that composites may offer a path to improved performance for other battery materials.

Hock Receives JUMP Award



Adam Hock, associate professor of chemistry and chemist in the catalysis group in the Chemical Sciences and Engineering Division at Argonne National Laboratory, received a Joint

University Microelectronics Program (JUMP) grant from the Semiconductor Research Corporation, with the University of Notre Dame as lead organization. The project was proposed over five years to develop new chemistry and precursors for the fabrication of next-generation semiconductor devices. The current award is for \$131,526.

Andrey Rogachev Distinguished Guest Speaker at the University of Kentucky

Andrey Rogachev, assistant professor of chemistry, was the Brown and Williamson Distinguished Guest Speaker on September 28 in the Department of Chemistry at the University of Kentucky-Louisville. Rogachev's talk on "Quantum Chemistry at IIT" outlined his research group's activities over the past five years. Among other topics, he explored the group's contribution to the chemistry and physics of polycyclic aromatic compounds with different surface topology and construction of supramolecular aggregates with pre-determined properties—creating prospective materials for batteries and spintronics. They have also contributed to the chemistry of early- and late-transition metals as well as analyzing and solving the problem of spin-states, which is one of the main problems of modern experimental coordination chemistry. A problem such as this can only be solved

by using an efficient combination of experimental and theoretical tools. Rogachev also presented a new area—the construction of a theoretical spectroscopic database for synthetic opioids—his group's response to the global synthetic drug epidemic.

To contact the Department of Chemistry, phone us at 312.567.3278 or email chemistry@iit.edu

Chemistry Ph.D. Candidate Elahe Moazzen Receives 2018 Crystallography Scholarship

Chemistry Ph.D. candidate Elahe Moazzen won a 2018 Ludo Frevel Crystallography Scholarship and will receive \$2,500 to assist in the continuation of her crystallographic research. She is one of 10 students awarded this year, selected on a competitive basis by the International Centre for Diffraction Data scholarship committee. Moazzen works in the Segre research group in the area of cost-effective, high-capacity alkaline battery research. The scholarship honors Ludo K. Frevel (1910–2011), who joined the Dow Chemical Company Spectroscopy Laboratory in 1936 and until his retirement, was one of Dow's top scientists.

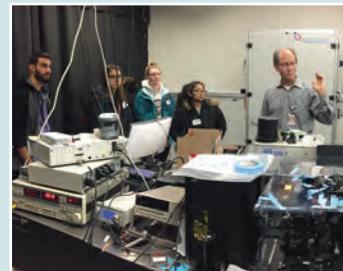


Siamak Shokri, Ph.D. candidate in chemistry in the Jean-Luc Ayitou research group, won a Best Poster Award at the 27th Inter-American Photochemical Society Meeting in Sarasota, Florida, January 2–5. Shokri won for his poster "Synthesis, Optoelectronic Properties and Excited State Dynamics of Baird-type Antiaromatic Thio- and Oxo-Naphthoquinodimethanes." Naphthoquinodimethanes are novel light-harvesting polycyclic molecular scaffolds, which have recently been synthesized in Ayitou's lab.

Spring 2018 Student Awards



[From left to right] Ph.D. candidates Elwin Clutter (TA Award), Shuyang Liu (Graduate Service Award), and Golbarg Mohammadiroozbahani (2017–18 Kilpatrick Fellow); Professor Carlo Segre, Interim Chair, Chemistry Department; Melisa Alkan (CHEM 4th year—Senior Award) and Abdallah Hasan (CHEM 3rd year—Junior Award).



Undergraduate Chemistry Club students visited the lab of Gary Wiederrecht in the Center for Nanoscale Materials Division at Argonne National Laboratory in March.

Looking Back

2018 Commencement

PHOTOS BY
PROFESSOR TOM IRVING



Congratulations to Our 2018–19 Kilpatrick Fellow

Elahe Moazzen, Ph.D. candidate

Fanta Award Recipients

Ph.D. candidate Elahe Moazzen gave a talk entitled “Lattice Templating and Galvanic Coupling Effects on the Electrochemical Performance of Core/Shell Battery Materials” at the 233rd Electrochemical Society Meeting held May 13–17 in Seattle.

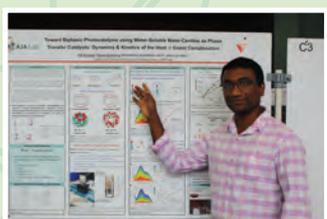
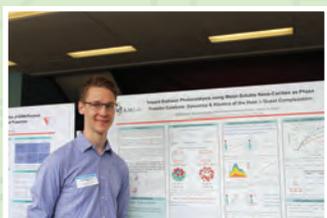
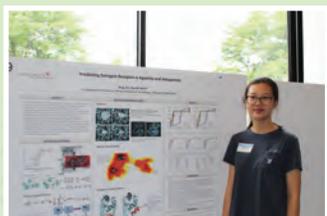
Ph.D. candidate Siyuan Ren attended the ACS Fall Meeting held August 19–23 in Boston. Ren won Best Poster at the Regional ACS Meeting on September 21.

Chemistry Poster Prize Winners

The following chemistry students won prizes at the College of Science joint-department event on August 16:

1st Prize Undergraduate:
William Blodgett
(CHEM 3rd year)

Poster Title: Toward Biphasic Photocatalysis Using Water-Soluble Nano Cavities as Phase Transfer Catalysts: Kinetic Studies of the Host: Guest Complexation (Advisor: Jean-Luc Ayitou)

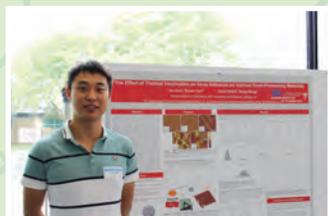
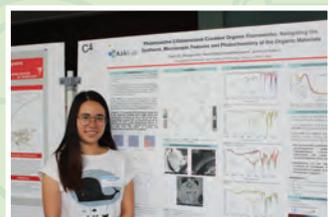
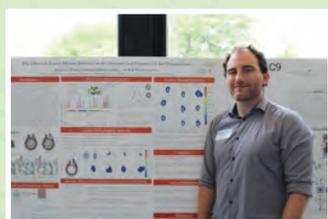


1st Prize Graduate:
Ph.D. candidate Golbarg Mohammadiroozbahani

Poster Title: Computation-Assisted Nanopore Detection of Thorium Ions (Advisor: Richard Guan)

2nd Prize Graduate: Ph.D. candidate Bing Xie

Poster Title: AI/GDock for Predicting Estrogen Receptor-Alpha Agonists and Antagonists (Advisor: David Minh)



Master of Chemistry in Materials Chemistry

Courtney Schrey, Sydney Smead

Master of Chemistry

Antao Gao, Wenlie Huang, Rui Ma, Divya Tadakamalla, Yinan Wang, Hua Xu, Shifang Yao, Yiqing Zhang

Master of Science in Chemistry

Chen Li received his M.S. degree in December 2017. His thesis title was "Computational Aided Structure-Function and Drug Design Analysis of Pathogenic Bacteria Membrane Proteins;" **Yiwei Lin** received his M.S. degree in May 2018 and completed his thesis on "Synthesis of New Cathode and Anode Structures for Lithium-Sulfur Batteries;" **Xiang Lu** graduated in May 2018 with a thesis on "Corannulene $\eta(\text{eta})^5$ -Coordination with Transition Metals: A Theoretical Study;" and **Zirui Zhang** received her M.S. in December 2017 on "Bonding Situations of N-Heterocyclic Carbenes and Its Heavier Analogs with Metal Complexes."

Ph.D. in Chemistry

Michael Foody graduated in May 2018 with a dissertation on "Precursor Chemistry: How the Chemical Properties of Precursors Drives the Synthesis of Nanoparticles and Nanofilms." **LaSalle Swenson** received his Ph.D. in May 2018 and did his dissertation on "Electroactive Colloidal Materials Derived from Polyoxometalates." **He Zhang** received his degree in December 2017 on "Synthesis and Reactivity of Organometallic Vapor Precursors in Depositin Thin Film Materials." **Xiaohan Chen** received his degree in August 2018 with a dissertation on "Nanopore-Based Nucleic Acid Detection." **Naiwei Chi** graduated in August 2018 with a dissertation on "Matrix Mediated Fibroblast Cell Stimulation to Promote Collagen Production for Connective Tissue Regeneration."

Where Are They Now?

Melisa Alkan was accepted into the chemistry Ph.D. program at Iowa State University.

Xiaohan Chen and Michael Foody were appointed as senior research associates (the former in the Guan research group; the latter in the Hock research group).

Yiwei Lin is a chemist in a Li-ion battery research development group at Apple Computers, PR China.

Siamak Shokri is chief scientific officer at CBGo Lab, LLC in Glenview, Illinois.

Yinan Wang is at the University of California-Riverside pursuing her Ph.D.

Yiqing Zhang was accepted into the chemistry Ph.D. program at the University of Georgia in Athens.

He Zhang is now working as a process engineer at Lam Research in Fremont, California.

2017–18 Degree Conferrals

Bachelor of Science

Melisa Alkan, Carlos Bustamante, Akena Latigo, Nicholas Politis, Yinan Wang

Master of Chemistry in Analytical Chemistry

Abigail Castillo, Jamie Dougherty, Kerry Fuller, Gordon Haring, Taylor Justice, Aaron Lavinder, Tri Le, Bertil Nshime, Nicole Pellicchia, Erena Sawyer Wagner, Kristin Corcoran, Colette Eusey, Ryan Koenes

Department of Chemistry

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



New M.S. in Analytical Chemistry

Illinois Tech's Master of Science in Analytical Chemistry is a new non-thesis master's degree (formerly, Master of Chemistry) designed for professionals working in the chemical industry, education, or government. The curriculum provides students with a solid foundation in separation science, spectroscopy, physical characterization, and method development. Our degree also emphasizes communication, industrial leadership, statistics, and business principles, which are essential for a scientific career in the business world.

All classes may be taken online, offering flexibility to complete the master's degree while working fulltime. As an option, a one-week practical laboratory class may be taken in Chicago with Lee Polite, adjunct faculty member and founder and president of Axion Analytical Labs.