CHEMISTRY ELEMENTS
A publication of the Department of Chemistry at Illinois Tech

Fall 2017
Welcome to the fifth annual issue of *Chemistry Elements*. By this time next year, you will be hearing from a new chair of the Department of Chemistry. An external search was initiated in August 2017 and the department will be busy visiting with top candidates over the next academic year. The entire department is anticipating the first new senior faculty hire in many years and an individual who can lead the department into the next decade. The new chair will also be working with a new dean of the College of Science. Russell Betts is stepping down after 10 years of service and will be serving as interim provost, and he leaves a strong college with more undergraduate majors than ever.

The new administrative team will be anticipating growth in the undergraduate chemistry major population due to the five new innovative degrees that the department developed and had approved by the Illinois Institute of Technology Board of Trustees. With these five new degrees—in environmental chemistry, forensic chemistry, bioanalytical chemistry, computational chemistry and biochemistry, and medicinal chemistry—we are taking advantage of our core strengths and providing our graduates with not only a rigorous B.S. degree in chemistry, but also a specialization that will provide them with a head start in a specific career. Please take a look at these new degree programs on our web page (science.iit.edu/chemistry/programs) and recommend them to any budding chemists who are interested in the kind of outstanding education that Illinois Tech can provide.

This past year, seven bachelor of science degrees and 34 master’s degrees were conferred. The majority of our new B.S. graduates have gone on to pursue advanced degrees.

After 22 years in the Robert A. Pritzker Science Center (formerly the Life Sciences Building), the departments of biology, chemistry, and physics now have the entire building to themselves after the relocation of the Department of Psychology in August 2017. As a first step in reconfiguration, the chemistry department office has moved into a newly remodeled suite—The Robert E. Frey Jr. Chemistry Suite—thanks to a generous donation from Bob Frey (CHEM ’65). We are looking forward to additional renovations, including new office space for teaching and research assistants, an ample student lounge, and room for expansion in faculty offices and laboratories. In addition the building will accommodate the newly established Center for Interdisciplinary Scientific Computation (CISC) and the College of Science dean’s office, which will be moving from the John T. Rettaliata Engineering Center over the next 12 months.

We are happy to welcome two new chemistry lecturers to Illinois Tech. Katie Leight and Somdev Banerjee started teaching for us in the fall 2017 semester. Katie recently completed her Ph.D. at Arizona State University, while Somdev graduated from Oregon State University. Both of them have an organic chemistry background and formal training in chemistry education.

In this issue, we are pleased to feature the research of A. Jean-Luc Ayitou, assistant professor, our organic chemist working in the area of photochemistry. He has developed an impressive lab since his arrival at Illinois Tech. Also in other research news, Richard Guan, associate professor, was awarded a three-year, $360,000 grant from the National Science Foundation for his project developing next-generation biomaterials.

At the end of this academic year, I will be stepping down as interim chair and handing the administration of the department over to the new chair. While I will no longer be involved in the day-to-day operations of the Department of Chemistry, I will still be in the same building, and I am going to be watching with interest as the department grows under its new leadership. It has been a pleasure for me to be able to serve the department in this transitional period.

**Carlo Segre**
*Interim Chair, Department of Chemistry*
*Duchossois Leadership Professor*
*Professor of Physics*
Novel Organic Light-Harvesting Compounds for Photonic Applications

Assistant Professor A. Jean-Luc Ayitou develops new strategies to create novel organic chromophores (light absorbing/emitting chemical entities) and materials, for applications ranging from solar energy to sustainable chemical syntheses. Research in the Ayitou lab is strongly interdisciplinary—blending a conventional approach from synthetic organic chemistry synthesis methods with photophysical and photochemical paradigms. Using these cutting-edge techniques and state-of-the-art instrumentation, Ayitou's lab aims to understand intra- and intermolecular interactions in the condensed phase of the new organic chromophores of interest.

Ayitou did his graduate and postdoctoral training in organic chemistry, photochemistry, photophysics and solid-state spectroscopy. His current research interests span photon upconversion, to energy transfer in organic crystalline solids, to patterning of 2-D organic polymers. His group recently published a paper on photon upconversion in the Journal of Physical Chemistry (ACS). Ayitou et al. devised a novel anti-aromatic light-harvesting sensitizer, which was used for the photon upconversion research. This is the first example of photon upconversion using an anti-aromatic triplet sensitizer that is structurally complementary to the emitter perylene, a highly fluorescent, yellow crystalline aromatic hydrocarbon.

Upconversion (or conversion of low-energy radiation to higher energy light particles) is an elegant and sustainable photon management approach that can help to maximize the efficiency of current photovoltaic (PV) devices. PV devices are solar cells that can absorb light and produce electricity. Ayitou is using polycyclic anti-aromatic compounds (PAAC) as light-harvesting antennae for photon upconversion research. He is also exploiting the outstanding photophysical properties of PAAC to sensitize polycyclic aromatic hydrocarbons (like perylene) for the design of next-generation organic photonic materials. These novel materials can be further derivatized to engineer high-efficiency photovoltaic devices and can be used for biological imaging in medicine.

Ayitou works with photoluminescence (the emission of light) wherein the organic materials he is developing can beget high-energy light upon absorption of low-energy radiation. For example, in biological imaging, red light can penetrate our tissue but cannot help in in vivo imaging because it is not high enough in energy to cause luminescence. A recent acquisition in Ayitou’s lab is an emissions spectrophotometer, used to visualize and quantify the photochemical upconversion phenomenon. The figure shows what upconversion looks like, where green photons are transformed into blue radiation.

Compared to aromatic molecules that can be extracted from natural feedstocks (e.g., crude oil and coal), anti-aromatic compounds are not commonly found in nature and are difficult to stabilize or synthesize, although they share some characteristics with their aromatic counterparts. Ayitou explains, “The synthesis of stable anti-aromatic compounds is challenging … only a handful of molecular systems exhibiting such a characteristic have been reported! What makes them a topic of interest for scientists is that they have very interesting photophysical properties.” Ayitou has synthesized anti-aromatic chromophores and has demonstrated PAAC are useful and ideal sensitzers for photon upconversion research, because (a) they gain aromaticity (or become aromatic) upon absorption of light and (b) they are structurally compatible with polycyclic aromatic hydrocarbons that exhibit outstanding photoluminescence properties.

Another focus of the Ayitou lab is on 1-D/2-D hybrid polymeric materials to study the dimensionality of solid-state photochemical reactions, energy propagation, and quantum chain reactions. A potential application that would emanate from the research involving these polymeric materials is the development of bio-compatible materials and vehicles for drug delivery. Ayitou looks forward to purchasing a Fourier-transform infrared spectroscopy microscope to analyze the microscopic structures of polymers. Visualizing and understanding the microscopic features of these organic materials will help in the better design and synthesis of their basic molecular building blocks.

Apart from setting up a well-run research lab and a very active group since his arrival at Illinois Tech, Ayitou is also enthusiastic about educating and mentoring undergraduate students who have a strong desire to pursue postgraduate education in the STEM disciplines (science, technology, engineering, and mathematics). Through Ayitou's outreach program, underrepresented undergraduate students can perform cutting-edge research under his supervision and with other colleagues in the College of Science. Furthermore, these students will receive unique mentoring in professional networking, teamwork, and leadership skills that will help propel them through their future endeavors.

Analytical Chemistry Program Celebrates 20th Year

On March 6, in the Robert A. Pritzker Science Center auditorium, more than 60 people joined the Department of Chemistry to celebrate the 20th anniversary of the professional master’s program in analytical chemistry. Carlo Segre, interim chair, gave Walter Eisenberg, professor emeritus and former chair of chemistry, a service excellence award for his vision in founding the successful program 20 years ago. Diep Nguyen, industry professor of chemistry and current director of the program, tied the event to the Pittcon Conference & Expo at McCormick Place, giving many of our professional chemistry alumni the opportunity to attend, and also coordinated the event to coincide with the students’ final oral exams on that day.

Tara Nylese (M.A.S. ACHM ‘12), returned to Illinois Tech to speak at the event. She is now a manager for EDAX Global Applications, and gave this advice to the students: “If you are not doing what you love, change gears. Once you find that [what you love], stick to it and be steadfast.” Nylese showed the audience how physical characterization as well as quantitative analysis and spectroscopy fit into her corporate work.

David Boldridge, lecturer and advisory board member,
gave an industrial chemist’s perspective as he occasionally hired new graduates at Cabot Microelectronics. He argued that whether one is an R&D analyst or is in quality control, sales, or manufacturing, each of these industry-specific areas requires a certain skill set. Recent graduates have only been given an introduction, he noted, yet the analytical chemistry master’s degree helps them build focused expertise in a rapid way.

Chris Latoz (M.A.S. ACHM ‘98), manager of stability and analytical services at Hollister Inc., spoke about how Eisenberg taught him organic chemistry using a challenging, nearly 2,000-page textbook, and he remembered Eisenberg’s great, clear teaching style. The program, he said, required 20 hours’ time commitment on top of a 40-hour-plus workweek. But his dedication paid off, and in December 1998, Latoz was in the first graduating class of the program. Members of the chemistry department were able to use this event to express their deep appreciation for Eisenberg’s service as well as Nguyen’s. With the latter’s commitment over the recent years, the program has seen a steady enrollment of about 50 students each year. This past spring, Nguyen launched a new intensive lab course, CHEM 700, which allowed students to gain hands-on training at Axion Analytical Labs in Chicago, a premier chemistry training facility.

Eisenberg recalled how years ago one student told him: “You have given me my life back,” removing a 50-mile commute to her university and creating more family time with the online lectures to view at home. “That is the beauty of the program,” Eisenberg remarked. “We have done a good thing.”

New Chemistry Lecturers

Katie Leight joins the Department of Chemistry as a lecturer, and she will also manage the organic chemistry laboratories. She obtained a Ph.D. in chemistry from the University of Arizona (2017), where she studied organic photovoltaic materials. Leight also was named a Distinguished Teaching Assistant for her work in organic chemistry and obtained a Certificate in College Teaching.

Somdev Banerjee joins the Department of Chemistry as a lecturer. He most recently taught general chemistry and organic chemistry at Linn-Benton Community College in Oregon. Banerjee obtained a Ph.D. in organic chemistry at Oregon State University (2017), where he studied synthetic organic chemistry. He also completed a Graduate Certificate in College and University Teaching.
Department of Chemistry Introduces Five New Majors

The Department of Chemistry has announced five new majors to help make students better candidates for in-demand graduate programs and jobs:

- B.S. in Environmental Chemistry—the first of its kind in Chicago
- B.S. in Forensic Chemistry—the first of its kind in Chicago
- B.S. in Bioanalytical Chemistry—the first of its kind in the country
- B.S. in Computational Chemistry and Biochemistry—the first comprehensive computer-related chemistry and biochemistry program in the country
- B.S. in Medicinal Chemistry—the first of its kind in Illinois, and one of only a handful in the country

These new degrees are designed to help students start to prepare for specific career paths, be more competitive in pursuing graduate programs and professional jobs, and learn skills that many other undergraduate programs do not offer.

The programs include opportunities to do research with faculty in such areas as biosensor technology for monitoring of pollution, green chemistry, biosensors for detection of bioterrorism chemicals and toxins, antibody drug conjugate chemistry, quantum chemistry, and drug discovery.

Student News

Chen Li, Master of Science candidate in the research group of Assistant Professor David Minh, was selected as an Outstanding Young Researcher at the workshop “From Computational Biophysics to Systems Biology (CBSB2017),” May 18–20 in Cincinnati.

The following students received Fanta Award funding to attend conferences:

Chen Li, Master of Science candidate—Biophysical Society 61st Annual Meeting in New Orleans, February 12–15

Melisa Alkan (CHEM 3rd year)—ACS Meeting in San Francisco, April 2–6

Qi Xu, Ph.D. candidate—ACS Great Lakes Regional Meeting in Fargo, North Dakota, June 27–30

Xiang Lu, Master of Science candidate—ACS National Meeting in Washington, D.C., August 20–24

Congratulations to Our 2017–18 Kilpatrick Fellow

Golbarg Mohammadiroozbahani, Ph.D. candidate and 2017–18 Kilpatrick Fellow

2016–17 Degree Recipients

Bachelor of Science in Chemistry: Yanda Chen, Paloma Corro, Nathan Donahue, Jomana Hatahet, Fazrurnaguib Paharuddin, James Tufts, Dan Yin, Haojie Chi, Tong Fan, Han Li, Jia Liu, Komil Dilbagh Singh Sandal, Divya Tadakamalla, Ruiqi Xie

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Our Alumni: Where Are They Now?

Yanda Chen (CHEM ’17) was accepted into our Ph.D. program and is working in the Chong lab.

Dan Yin (CHEM ’17) is a first-year graduate student in the chemistry department of the University of Wisconsin-Madison.

Nathan Donahue (CHEM ’16) is working as a research technician in the Irvine Lab at Massachusetts Institute of Technology.

Paloma Corro (CHEM ’16) is pursuing her master’s degree in science education in the Department of Mathematics and Science Education at Illinois Tech. She has been student-teaching in the Chicago Public Schools on the path to becoming a high school chemistry teacher.

Joanne Gucwa (CHEM ’68) was featured in the spring 2017 issue of IIT Magazine for her science-based children’s books.

Chemistry’s Guan Receives $360,000 NSF Award for the Study of Nanopore-Based MMP/ADAM Profiling for Early Cancer Detection

Associate Professor Xiyun “Richard” Guan has received a three-year, $360,000 grant from the National Science Foundation for his project “Solid-State Nanopore-Based MMP/ADAM Profiling for Early Cancer Detection.” The award is to develop next-generation biomaterials to help detect and treat cancer.

Guan develops nanopore techniques for various applications in biotechnology at the single-molecule level. Nanopores are pores or cavities only a few nanometers in size. The NSF-funded research will make use of Guan’s innovations in nanopores to improve the understanding of MMPs (matrix metalloproteinases) and ADAMs (short for a disintegrin and metalloproteinase), both enzymes known to be part of cancer invasion and metastasis. Scientists have become greatly interested in these as providing clues to cell health and potential targets for early detection and treatment of cancer. To date, however, MMP/ADAM assays have not been selective or sensitive enough.

Guan’s work will help address that problem. He will use his nanopores to do highly selective and sensitive measurement of the activity of MMPs/ADAMs, and develop a portable multiplex nanopore sensing system to profile MMPs/ADAMs in human serum. Such a sensing technique not only can provide precise diagnosis of cancer type and cancer stage, but also has a potential application in cancer therapy. In addition, the proposed studies are expected to lead to a better understanding of molecular and ionic transport, as well as to develop a versatile tool for various applications, including biosensing, studying covalent and non-covalent bonding interactions, investigating biomolecular folding and unfolding, and exploring enzyme kinetics.

Professor Hyun-Soon “Joy” Chong was featured last fall in IIT Magazine for her research in the area of immunotherapy. Chong is developing antibody drug conjugates for targeted cancer therapy. She was also instrumental in developing the new chemistry programs this year, tailored for five different career paths.

Associate Professor Xiyun “Richard” Guan received a new award from the National Science Foundation (see feature story). Guan also received a $422,500 three-year renewal award from the National Institutes of Health to continue his project “Label-Free Nanopore Biosensor for Rapid, Ultrasensitive, and Multiplex Detection of Protease Activities.”

Associate Professor Adam Hock continues his joint appointment in the Catalysis Group in the Chemical Sciences and Engineering Division of Argonne National Laboratory. He continues to serve as secretary for the Illinois Tech University Faculty Council. In addition to publishing eight peer-reviewed research papers in 2016, he helped to organize workshops sponsored by the National Science Foundation and the United States Department of Energy. He also worked with other university faculty (Andrew Howard, associate professor of biology and physics and interim chair, biology, and Jeff Wereszczynski, assistant professor of physics) to run a program in collaboration with the Academy for Urban School Leadership and National Louis University to help prepare Chicago Public School teachers for the more demanding design-based research approach to teaching science.

Professor M. Ishaque Khan, director of the Master of Chemistry in materials chemistry program, is pursuing collaborative research during his sabbatical this year at Argonne National Laboratory in the area of nanoscale materials and water science and engineering. His goal is to develop functional materials and composites for new and inexpensive technologies to monitor toxic chemicals and clean water. Khan presented some of his research in the keynote address “Functional Nanomaterials: Potential and Promise in Catalysis and Gas Sensing” at the International Conference on Catalysis and Chemical Engineering, February 22–24, in Baltimore. His recent publications include articles in Inorganic Chemistry Communications (2017) on “Novel Colloidal Materials from Functionalized Polyoxometalates” and in Solid State Sciences (2017) on “Structure-Property Relationships in NOx Sensor Materials Composed of Arrays of Vanadium Oxide Nanoclusters.”

Professor Braja Mandal received a $30,000 Wanger Institute for Sustainable Energy Research (WISER) award for his project “Monolithic Electrodes Made of Nanostructured Materials to Advance Li-S Battery Technology.”

Assistant Professor David Minh gave invited talks at: “Recent Advances in Modelling Rare Events” (RARE2017) conference in Agra, India, December 7–10; the workshop “Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics,” held at the Telluride Science Research Center, Telluride, Colorado, July 11–15; and the workshop “Beyond Kds: New Computational Methods to Address Challenges in Drug Discovery,” at the Centre Européen de Calcul Atomique et Moléculaire, Ecole Polytechnique Fédérale de Lausanne, Switzerland, June 6–9.

The research groups of Minh and Oscar Juarez, assistant professor of biology, have discovered a new structural motif in an essential Vibrio cholerae enzyme that could lead to important drug development. David Minh’s article “Hamiltonian Monte Carlo with Constrained Molecular Dynamics as Gibbs Sampling,” co-authored with Laurentiu Spiridon, former senior research associate in his group, appeared in the Journal of Chemical Theory and Computation. Minh and Spiridon developed and applied a technique to use a time-saving method of constrained molecular dynamics in the simulation of molecular motions. In constrained molecular dynamics, certain motions are suppressed, allowing simulations to proceed more quickly.

Assistant Professor Andrey Rogachev’s research was featured on the frontispiece of Angewandte Chemie Int’l Edition (see cover). In an article in Chemical Science (Feb 2017), Rogachev described how he and his group performed an extensive theoretical modeling, which revealed that magnetic coupling between polyaromatic radicals in such supramolecular aggregates can be fine-tuned by using alkali metals of different sizes. This resulted in successful synthesis and isolation of different supramolecular aggregates.

Rogachev gave five invited talks including “One- and Three-Electron Bonding in Conjugated Hydrocarbons” at the 253rd American Chemical Society National Meeting & Exposition, San Francisco, April 2–6; “Mechanism of Oligomerization of N-Heterocyclic Silvlenes into Zwitter-Ionic Silenes” at the 48th Silicon Symposium, Philadelphia, June 7–9; “Supramolecular Chemistry of Highly Reduced Buckybowls,” a symposium in honor of Nobel laureate Roald Hoffmann at the 254th ACS National Meeting, Washington, D.C., August 20–24; and “Triianionic Corannulene: Tuning Stability of Supramolecular Aggregates with Alkali Metal Size” at the 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany, August 27–September 1.

Professor Carlo Segre, Duchossois Leadership Professor of Physics and interim chair of the Department of Chemistry, recently had his endowed chair renewed for another three-year term. The chair honors faculty who are exemplary in scholarship, education, and service.

In response to Volvo announcing that all of its new cars will be either hybrid or electric by 2020, Segre was interviewed on WBEZ radio on July 17 for his expertise in the area of battery research and the future of electric cars.
Research Associate Professor Elena Timofeeva was featured last fall in Huffington Post, Phys.org, and American Inno for her company AquaGrow Technologies, founded with John Katsoudas (PHYS '96, M.S. ‘03), senior research associate in physics. AquaGrow is dedicated to designing and building fully containerized mobile aquaponics farms that will use local food waste instead of electricity as the energy source. This novel approach will enable a more profitable and grid-independent farming model for indoor food production, which is becoming increasingly needed because of global climate change and a growing population.

Professor Rong Wang received three awards during the past year: (1) an Illinois Tech innovation grant for collaborations to re-establish the International Center for Sensor Science and Engineering; (2) as co-PI with the Institute for Food Safety and Health for the United States Food and Drug Administration grant project “Assessing the Strength of Virus Adhesion on Food Contact Surfaces and the Effect of Food Processing on Virus Adhesion”; and (3) a grant from the Institute for Translational Medicine (NIH consortium) with Sylvia Botros, M.D. at the NorthShore University HealthSystem on the “Role of the Integration of Tissue Components in Pelvic Floor Tissue Biomechanics Associated with Pelvic Organ Prolapse.” Wang’s group recently published in ACS Omega, 2017, 2 (6), on their work to optimize the condition of glutaraldehyde treatment of collagen-silk composite fibers to achieve effective control and fine-tuning in tissue engineering applications.

Successful 2017 Kilpatrick Lectures Focused on Sensor Science

The 2017 Kilpatrick Lectures were held April 10 in Hermann Hall. The focus was on “Sensor Science and Technology,” a highly interdisciplinary field with important applications across all areas of chemistry and chemical engineering. Sensor science promises beneficial effects for the environment, biomedicine, and analytical and physical organic chemistry. We were pleased to have three distinguished speakers:

1. Eric Anslyn from the University of Texas at Austin gave an analysis of how organic chemistry can be used to mimic the senses of taste and smell.

2. Rashid Bashir, a pioneer in the field of bionanotechnology from the University of Illinois at Urbana-Champaign, spoke on bioMEMS (microelectromechanical systems) biomedical nanotechnology and presented his work on four different detections and developments.

3. Frances S. Ligler, jointly from the University of North Carolina at Chapel Hill and North Carolina State, spoke on the keys to biosensor sensitivity. Drawing from biosensors developed in her lab, she provided examples of how manipulating elements increased (or decreased) sensitivity for target analytes.