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CHEMISTRY ELEMENTS

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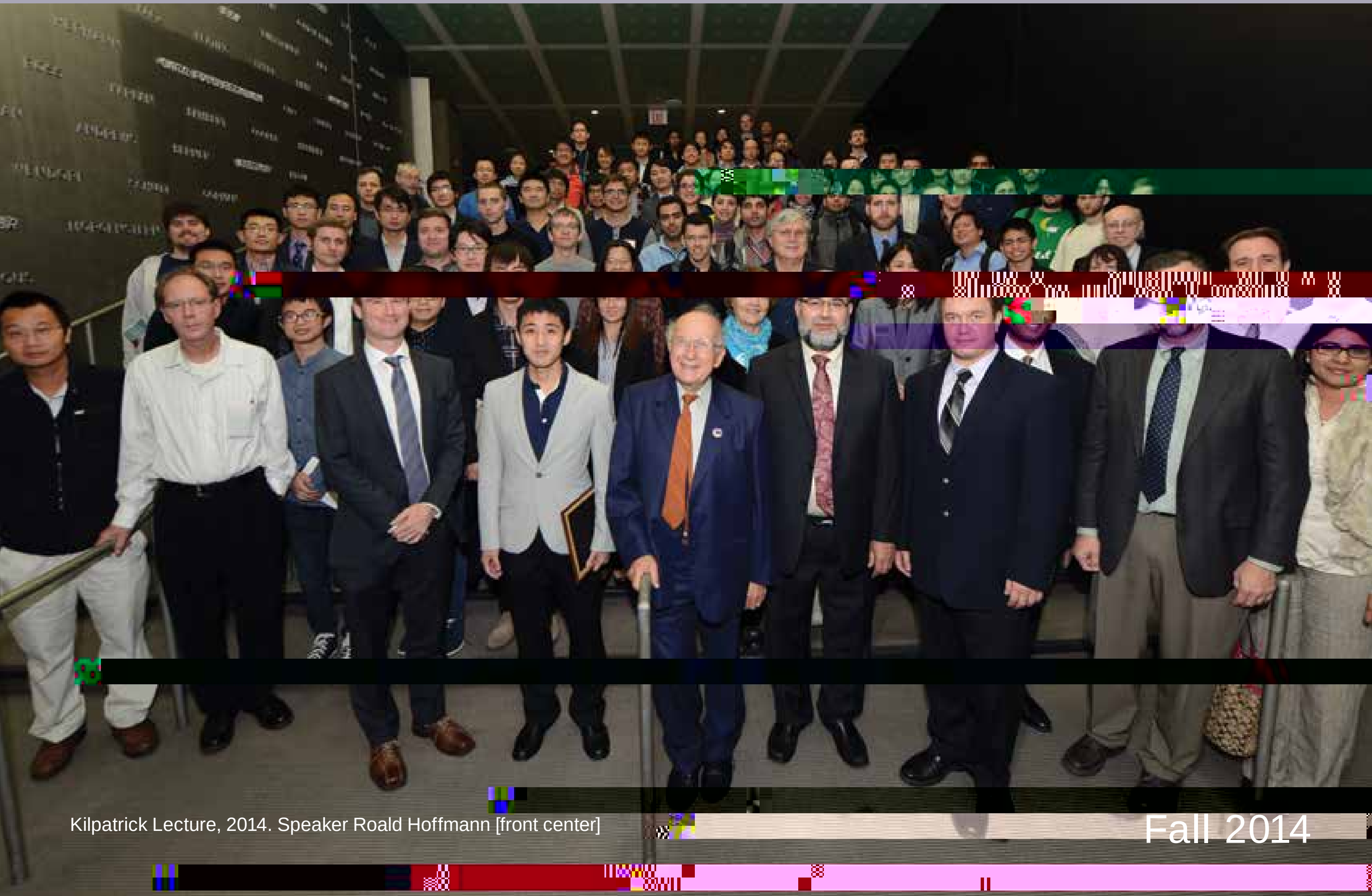

Kilpatrick Lecture, 2014. Speaker Roald Hoffmann [front center]

Fall 2014

We are pleased to present our second issue of *Chemistry Elements,* the newsletter of IIT Chemistry. This issue celebrates our recent developments as we prepare for our formal

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The contemporary problems of the world include developing affordable healthcare and nding sustainable solutions to the staggering energy needs of society. At IIT Chemistry, we are interested in both of these areas. In our last issue, we explored some of the energy research conducted in the department. Here, we present the work of several faculty members who are carrying out research work in the area of biological chemistry in the context of healthcare. This includes interdisciplinary research projects aimed at developing safe, effective, and targeted drugs for cancer and neurodegenerative diseases. Additionally, efforts are under way to discern how the microenvironment impacts stem cells for potential application in regenerative medicine. Chemistry faculty are also employing state-of-the-art computational chemistry methods for drug discovery. Following is an overview of some of the department research in this eld.

A [illegible] is working on the development of biosensors for detecting environmental toxins and biomolecules using nanopore sensing. A nanopore is a nanoscale cavity or channel, sometimes created by a pore-forming protein. When a nanopore resides in a membrane, only single molecules can pass through the pore, and as a result the pore acts as a single-molecule detector. Over the last 15 years, these nanoscale pores have been used not only to analyze the sequence of DNA, but also to study various types of chemical interactions. They have been used to investigate biomolecular structure, for example the folding and unfolding of proteins, and for other applications.

As an emerging technique, nanopore sensing has many advantages over existing techniques, including real-time detection. It also does not require the use of uorescent dyes or radioactive materials; therefore, it is known as a label-free technique. Nanopore sensing has the ability to detect ultra-low concentrations of analytes (targeted species), for example trace amounts of biomolecules as found in human blood samples. Nanopore sensors can detect the concentration and identity of an analyte based on the ionic current modulations in a salt solution. When the molecules of interest, such as peptides, proteins, or DNA (with diameters smaller than the nanopore) pass through a single nanopore, they will produce current modulations for analysis.

One aspect of Guan's nanopore research is centered on pioneering a new, highly selective and sensitive technique to measure the activities of proteases, which are enzymes that break down proteins and peptides (short amino acid chains). Proteases occur naturally in all living organisms and play key roles in diverse biological processes, from cell regeneration and metastasis to cell deterioration and immune defense. Accordingly, alterations in the structure and expression patterns of proteases underlie many human pathological processes including cancer, arthritis, osteoporosis, in ammatory disorders, and neurodegenerative, cardiovascular and autoimmune diseases. Thus, proteases may serve as valuable diagnostic or prognostic markers for disease states, and are becoming increasingly important targets for drug discovery.

Nanopore measurement of protease activity is achieved by real-time monitoring of the cleavage of a peptide. As shown at the top of Figure 1, when there is no presence of a target protease, peptide molecules pass through the nanopore giving one signal reading. By contrast, at the bottom of the gure, if a protease is present in a solution and, acting like a scissors, cuts the peptide molecules, the cleavage products produce entirely different current modulations. A comparison of the readings quanti es protease enzymatic activity.

The real-time, label-free nanopore sensing technique discovered in this project should nd useful application in the detection of proteases of medical or biological importance.

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works on developing

[illegible], lecturer in chemistry, joined us for the 2014-15 academic year. Gothard received her Ph.D. in chemistry from Northwestern University in 2013, where her research was focused on computer-assisted design, prediction, and the development of novel tandem chemical pathways to medicinally important quinoline scaffolds and inhibitors used in anti-asthma treatment. Prior to Northwestern, she worked at the University of California, Irvine, as a research assistant, where she pursued projects involving solid-phase synthesis of unnatural peptides and the development of unique intramolecular uorescent energy transfer assays. Gothard's postdoctoral research was at the University of Chicago, where she worked to develop biocompatible surfactant polymers to seal cell membranes and refold denatured proteins. Her interests include chemical education, scienti c management, medicinal chemistry, and organic syntheses.

[illegible] has been promoted to full professor beginning in the 2014-15 academic year. She has been very successful in receiving continued funding from the National Institutes of Health and has active research programs related to the development of cancer therapeutic and diagnostic drugs.

A [illegible] received a grant award from the National Institutes of Health for his project entitled "Label-Free Nanopore Biosensor for Rapid, Ultrasensitive, and Multiplex Detection of Protease Activit- a gave a keynote lecture entitled "Functional Nanomaterials: Potential and Promise for Addressing Current Technological Challenges" at the International Conference on Nanoscience and Nanotechnology, in Aligarh, India, March 8-10.

gave invited talks at the following meetings in May: The International Symposium at the Vasundhara Sarovar Premiere in Vayalar, Kerala, India; Biological Physics Seminar at Northeastern University in Boston, Mass.; The Harvard-MIT Universities Allied for Essential Medicines student organization, at Harvard Medical School in Boston, Mass; and a workshop at Vertex Pharmaceuticals in Boston. Minh also gave a talk at the Molecular Recognition Workshop at the Telluride Science Research Center in Telluride, Colo., on August 11-15, and at the Midwest Enzyme Chemistry Conference at Northwestern University on Sept. 27.

chaired the section on Molecular Design at the International Conference on Chemical Bonding, July 24-28, in Kauai, Hawaii, and gave a talk entitled "Sandwich-like Aggregates of Highly Reduced Corannulene: Theoretical Study of Their Formation and Electronic Structure." Rogachev also gave a talk at a conference near Casablanca in Morocco, Sept. 22-25, on theory and prediction of sandwich-like aggregates of buckybowls.

gave a talk entitled "Collagen-based Nanocomposite Materials and Their Roles in Stem Cell Differentiation" at the International Conference on Composites/Nano Engineering (ICCE-22) in Saint Julien, Malta, July 13-19.

, assistant professor of chemistry and assistant scientist at Argonne National Laboratory (ANL), and colleagues at ANL and Northwestern University have developed a new catalyst to transform propane into propene (propylene).

Propene, with worldwide sales of $90 billion in 2008, is a crucial product for the petrochemical industry, used in the manufacture of plastics, packaging and other applications. Current catalysts, while very active for the production of propene, also produce methane and ethylene (smaller hydrocarbon fragments) through unwanted side reactions. Separating the desired products adds to the energy demand and cost of the process. The new catalyst, a silica supported single-site Zn(II) catalyst, is more selective for the desired propane to propene transformation, Roald Hoffmann, who received the Nobel Prize in chemistry in 1981, delivered the 2014 Kilpatrick Lecture on Monday, September 15, in the McCormick Tribune Campus Center (MTCC) Auditorium. A poster session followed the lecture, exhibiting some of the ongoing research in chemical sciences at IIT, along with a reception. This was the second time that Hoffmann was selected; he also gave the lecture in 1973 and is one of seven Nobel Laureates to deliver the prestigious Kilpatrick Lecture.

The event was attended by students, faculty, alumni, and guests from various universities, Argonne National Laboratory, and industry. After welcome remarks from Chairman Khan, President Anderson spoke, and Assistant Professor Andrey Rogachev, former post doc in Hoffmann's research group, introduced the speaker.

In his lecture, "All the Ways To Have a Bond," Hoffmann gave an overview of how people look at chemical bonds, from both the theoretical and experiential perspective. Earlier in the day, students and faculty enjoyed a breakfast with Hoffmann in the department, hearing stories about his past, about the Nobel Prize, and interesting perspectives on the history of chemistry, the impact of modern technology on the discipline, and what the future holds.