#### **Event Schedule**

| 3 p.m.    | Welcome from Chemistry Executive Associate Chair M. Ishaque Khan  | 4:15 p.m. | Intermission  |  |
|-----------|---|-----------|---|--|
| 3:05 p.m. | Remarks from IIT College<br>of Science Dean Russell Betts   | 4:30 p.m. | Part II,<br>All the Ways to Have a Bond   |  |
| 3:10 p.m. | Introduction of the speaker,<br>Roald Hoffmann, by Assistant<br>Professor of Chemistry Andrey<br>Rogachev, chair of the Kilpatrick<br>lecture committee | 5:30 p.m. | Kilpatrick fellowship and<br>Kilpatrick scholarship awards,<br>Professor M. Ishaque Khan                    |  |
| 3:15 p.m. | 2014 Kilpatrick Lecture:<br>Roald Hoffmann,<br>Frank H.T. Rhodes Professor<br>of Humane Letters, Emeritus,<br>Cornell University<br>Part I,             | 5:45 p.m. | Reception and poster session,<br>MTCC Ballroom<br>Refreshments will be served; all<br>attendees are invited |  |
|           |   | 7:00 p.m. | Poster session awards,<br>Assistant Professor of Chemistry  |  |

## Past Kilpatrick Lecture Speakers

Brant Cage

All the Ways to Have a Bond

| 1966<br>1967<br>1968<br>1969 | Ronald Percy Bell<br>Lord Wynne-Jones<br>Henry Eyring<br>Martin Karplus<br>John D. Roberts | 1984<br>1985 | Symposium: Chemistry at Metal Surfaces Jack Halpern David L. Beveridge Symposium: Polymers (in memory of Paul Flory) | 1999 | K. C. Nicolaou Wolfgang Gopel Symposium: Computational Chemistry with John Pople |
|------------------------------|--|--------------|--|------|--|
|                              | Manfred Eigen,<br>George B.<br>Kistiakowsky  |              |  | 2001 | Symposium:<br>Nanoscience<br>and Nanotechnology                                  |
| 1971                         | John R. Platt  | 1989         | Jaqueline K. Barton  | 2003 | Barry M. Trost   |
| 1972                         | George C. Pimentel   | 1991         | Mark S. Wrighton   | 2004 | Symposium: Enzyme  |
| 1973                         | Roald Hoffmann   | 1992         | Symposium:   |      | Dynamics   |
| 1974                         | Richard B. Bernstein   |              | Conducting   | 2008 | Fraser Stoddart  |
| 1975                         | Henry Taube  |              | Polymers   | 2009 | Susan V. Olesik  |
| 1976                         | William N. Lipscomb  | 1993         | Mary Anne Fox  | 2010 | Symposium: Recent  |
| 1977                         | Melvin Calvin  | 1995         | Symposium:   |      | Advances in Polymer  |
| 1978                         | Symposium: Fast<br>Time Spectroscopy<br>and Chemistry                                      |              | Synchrotron<br>Radiation in<br>Chemistry   | 2011 | Science and Technology George Whitesides   |
| 1981                         | Symposium:<br>Carbenes,  | 1996         | Symposium: Host-<br>Guest Interactions   | 2013 | Daniel G. Nocera   |

IIT Chemistry presents

The 2014 Kilpatrick Lecture

# ALL THE WAYS TO HAVE A BOND



## **Roald Hoffmann**

Cornell University

The McCormick Tribune Campus Center (MTCC), McCloska Auditorium
IIT Main Campus, 33rd & State Street, Chicago
Monday, September 15, 2014



SCIENCE: THE RAW FUEL OF INNOVATION



Carbenoids,

Cyclopropanes

in Organic Synthesis

and

Supramolecular

Structures



Welcome to the 2014 Kilpatrick Lecture in chemistry. The theme of this year's Kilpatrick event is "All the Ways to Have a Bond." We are very excited to welcome back Roald Hoffmann, Frank H.T. Rhodes Professor of Humane Letters, Emeritus, at Cornell University, who was the Kilpatrick Lecturer 41 years ago in 1973 and returns to us as a Nobel laureate. Hoffmann received the 1981 Nobel Prize in Chemistry jointly with Kenichi Fukui for "their theories, developed independently, concerning the course of chemical reactions." His Woodward-Hoffmann rules are famous in organic chemistry. For inorganic chemists, his isolobal analogy principle is an extremely useful tool for

quick and reliable qualitative prediction and construction of electronic structures of new molecules on the basis of already known species. And computational chemists benefit from the extended Hückel approach, which made it possible to understand orbital interactions. Current research activities of Hoffmann cut across all fields of modern chemistry, with specific emphasis on bridging the gap between molecular and solid-state chemistry.

The legacy left by Martin and Mary Kilpatrick has continued to inspire innovative teaching and creative research at IIT. A prominent example is our chemistry program, which provides a rigorous education that competitively prepares our students for careers in academia, industry, and government. Our research programs cut across traditional areas of science to solve real-world problems in catalysis, pharmaceuticals, therapeutics, materials, and sustainable energy.

On behalf of the IIT chemistry community, faculty, staff, and students, and the lecture committee, I would like to thank you for joining us for this special IIT annual event. We hope you enjoy the program.

Sincerely,

M. Ishague Khan, Professor of Chemistry, Executive Associate Chair, Chemistry

## About the Kilpatrick Lecture



IIT's annual Kilpatrick Lecture honors Martin and Mary Kilpatrick, who were outstanding researchers and educators. Martin served as chair of IIT's Department of Chemistry from 1947–1960, leading the department to national prominence in both undergraduate and graduate instruction and research. As a scientist, Martin made his mark in fundamental chemical research in areas of physical and inorganic chemistry, and materials science. Mary was a chemistry faculty member from 1947–1964.

The Kilpatricks devoted their lives to the critical and creative study of chemistry, particularly chemical kinetics, acid-based reactions, and electrolyte chemistry. Before coming to IIT in 1947, Martin was a professor at the University of Pennsylvania and assisted Harold Urey in the Manhattan Project at Columbia University. Both Kilpatricks were Fulbright research scholars who studied in Denmark under the legendary J. N. Brønsted.

As chair at IIT, Martin guided the department during a period of vigorous growth and development in both teaching and research. Initially, the department occupied all of Wishnick Hall—one of the then three new buildings by Ludwig Mies van der Rohe that marked the beginning of today's modern Main Campus.

In recognition of the Kilpatricks's achievements at IIT, Martin's successor, Arthur E. Martell, and faculty colleagues instituted the now permanently endowed Kilpatrick Lecture.



Roald Hoffmann was born in 1937 in Złoczów, Poland. Having survived the war, he came to the U. S. in 1949, and studied chemistry at Columbia and Harvard Universities (Ph.D. 1962). Since 1965 he is at Cornell University, now as the Frank H. T. Rhodes Professor of Humane Letters, Emeritus. He has received many of the honors of his profession, including the 1981 Nobel Prize in Chemistry (shared with Kenichi Fukui).

Notable at the same time is his reaching out to the general public; he was the presenter, for example, of a television course in chemistry titled "The World of Chemistry," shown widely since 1990.

As a writer, Hoffmann has carved out a land between science, poetry, and philosophy through many essays and five books: Chemistry Imagined with artist Vivian Torrence; The Same and Not the Same (translated into six languages); Old Wine, New Flasks: Reflections on Science and Jewish Tradition, with Shira Leibowitz Schmidt; a book of his collected essays (edited by J. Kovac and M. Weisberg) Roald Hoffmann on the Philosophy, Art, and Science of Chemistry; and Beyond the Finite: The Sublime in Art and Science, coedited with lain Boyd Whyte. Five collections of his poetry have been published, including booklength selections of poems translated into Spanish (Catalista, Huerga y Fierro, Madrid) and Russian (Izbranniye Stichotvorenia, Tekst, Moscow). He has also co-written a play with fellow chemist Carl Djerassi, entitled Oxygen, and two by himself, Should've and Something that Belongs to You.

www.roaldhoffmann.com

### ALL THE WAYS TO HAVE A BOND

This lecture takes two hours, with an intermission.

The concept of a chemical bond, so essential to chemistry, and with a venerable history, has life, generating controversy and incredible interest. Even if (or maybe because) we can't reduce it to physics.

I will discuss some of the common experimental criteria for judging the presence and strength of a bond: length, energy, force constants, magnetism, energy splittings and other spectroscopic criteria. On the theoretical side, I will look at bond orders, population analyses, bond critical points, and electron localization functions. And will give a personal opinion on the utility of the various measures.

My advice at the end is likely to be: Push the concept to its limits. Think about any bond in terms of all the various criteria, experimental and theoretical, that we have discussed. Accept that (at the limits) a bond will be a bond by some criteria, maybe not others. Instead of wringing your hands about how terrible it is that this concept cannot be unambiguously defined, have fun with the fuzzy richness of the idea.

Try to understand what motivates other people to say there is a bond there or isn't. Always think about what change (chemical perturbation) you can do to probe your ideas.