

“In the past quantum chemists believed that their foremost duty was to develop approximate methods with which one could reproduce physical quantities that can be measured accurately. Obviously, it will always be necessary to check new theoretical methods but the principal duty is becoming more and more the computation of (in principle measurable) physical quantities which are not or not easily amenable to experiments (e.g., properties of short-lived species). It is increasingly the cost which determines whether one computes a given physical quantity or decides to measure it ...”

Ede Kapuy (1969)

Previous Ede Kapuy Lectures at the Institute of Chemistry,
ELTE Eötvös Loránd University, Budapest, Hungary:

2000	Henry F. Schaefer III	2011	István Mayer
2001	Rodney J. Bartlett	2012	Hans Lischka
2002	John F. Stanton	2013	Werner Kutzelnigg
2003	Josef Paldus	2014	Paul G. Mezey
2004	Debashis Mukherjee	2015	Paul Ayers
2005	Jürgen Gauss	2016	Trygve Ulf Helgaker
2006	Ingvar Lindgren	2017	Jerzy Cioslowski
2007	Mark Hoffmann	2018	Jean-Paul Malrieu
2008	Hiroshi Nakatsuji	2019	Markus Reiher
2009	Enrico Clementi	2021	Jozef Noga
2010	Wilfried Meyer		

22nd ANNUAL

**EDE KAPUY
MEMORIAL LECTURE**

Thursday, 5th of May, 2022
2:30 P.M. auditory 062 (Gróh room),
Institute of Chemistry
ELTE Eötvös Loránd University
1117 Budapest, Pázmány sétány 1/A

Barney Ellison

**Radical / Radical Reactions,
Conical Intersections, and the
Formation of Soot**

Presented by the
Laboratory of Theoretical Chemistry
ELTE Eötvös Loránd University, Budapest

EDE KAPUY (1928 – 1999)

Ede Kapuy was born on 21 September, 1928 in Győr (Hungary). His family directed him toward becoming a priest. This was perhaps due, in part, to the influence of his uncle, who had been a priest-teacher at the local Gergely Czuczor Roman Catholic Gymnasium of the Benedictine Order, whose presence in Hungary exceeds 1000 years. It is not surprising, therefore, that he attended the Czuczor Gymnasium.

After finishing high school, Ede Kapuy chose a different future from what his parents suggested by deciding to become a chemist and entering the Péter Pázmány University of Budapest, named after the founder of our university. He graduated in 1952 from the same institution, renamed in the meantime after Loránd Eötvös, the world-famous Hungarian physicist.

Ede Kapuy received his first higher degree in physics (Candidate of Physics) as a co-worker of Professor Pál Gombás at the Technical University of Budapest. In 1958 Ede Kapuy joined the Research Group for Theoretical Physics (later renamed the Quantum Theory Group of the Hungarian Academy of Sciences) of Professor Gombás. Ede Kapuy completed his second higher degree (Doctor of Physics) in 1971, became a senior research scientist, and eventually Professor of Physics in 1977. From 1983 he was a full professor of Theoretical Physics at the Attila József University of Szeged (Hungary).

Ede Kapuy was a member of the Physics Committee of the Hungarian Academy of Sciences and head of the Quantum Chemistry Group of the Hungarian Chemical Society. He was a fellow of the World Association of Theoretically Oriented Chemists (WATOC). Between 1981 and 1985 he served as a member of the Editorial Board of the Journal of Molecular Structure (Theochem).

The main contribution of Ede Kapuy to quantum chemistry is the development of the separated pair theory in the late fifties and early sixties. Later, his interest turned to the electron localization problem. He published 66 papers in English and 13 papers in Hungarian. He was author or co-author of 4 books, including perhaps the best Hungarian textbook on quantum chemistry, titled *Electronic Structure of Atoms and Molecules* (co-authored by Ferenc Török). He was a visiting professor at major universities in England, Germany, and Canada. He frequently served as a member of organizing committees of international conferences on quantum chemistry.

The academic interests of Ede Kapuy were not limited to his own field of research, quantum physics and quantum chemistry. His knowledge of physics at large was remarkably broad. His extensive reading was only surpassed by his extraordinary memory – if he declared that he had not read anything about a particular problem, it was unnecessary to check the literature. On the other hand, if he read something important about the topic, he could name not only the year but the location of the contribution.

The hobbies of Ede Kapuy included history and geography. He acquired such a distinguished knowledge in these subjects that he was considered an expert on these matters, as well.

The establishment of the Kapuy lecture series in quantum chemistry recognizes the contributions and legacy of this remarkable scientist.

BARNEY ELLISON

Barney Ellison taught Organic Chemistry at the University of Colorado at Boulder from 1977 – 2014. He is now Professor Emeritus and no longer teaches undergraduate classes. He still has an active research laboratory and collaborates with groups at Joint Institute for Laboratory Astrophysics (JILA), University of Florida, and Harvard.

Ellison took an undergraduate degree at Trinity College (Hartford, CT) where he was a pre-medical major. Upon graduation in 1965, he wanted to understand the action of antibiotic drugs in cells, so he matriculated to the Department of Pharmacology in the medical school at Yale University. Following two years of graduate work in Pharmacology, he switched to the easier subject of Chemistry. He studied for a Ph.D. in organic chemistry at Yale under the supervision of Professor Ken Wiberg and earned his degree in 1974.

In order to explore the dynamic correlation of electrons in organic molecules, Ellison accepted a postdoctoral appointment with Professor Bill Reinhardt. Reinhardt had just moved from Harvard out to JILA in Boulder, Colorado. While working with Reinhardt's group, he met Carl Lineberger and participated with the experimentalists in JILA to study the negative ion photoelectron spectroscopy of the simplest carbene anion, CH_2^- . Following his postdoctoral stay at JILA, the Department of Chemistry at the University of Colorado offered Ellison a faculty position as an Assistant Professor of Organic Chemistry. He was promoted to the rank of full Professor by the University of Colorado in 1988.

While at the University of Colorado, Ellison has developed a research program to study organic reactive intermediates. He uses negative ion photoelectron spectroscopy, matrix isolation FTIR spectroscopy, flowing afterglow SIFT mass spectrometers and photoionization mass spectrometers to study the dynamical properties of polyatomic organic ions and radicals. In later years, he has become interested in the atmosphere and the organic chemistry of aerosols. Aerosols are μm -sized atmospheric particles that trigger the formation of clouds. Because biomass burning is a major source of the carbon that is incorporated into continental aerosols, Ellison is beginning the study of the thermal cracking of biomass. The experiments on thermal decomposition of complex fuels and biomass are developed in collaboration with the Mechanical Engineers at the University of Colorado (Professor John W. Daily, Professor Nicole Labbe, Professor Hope Michelsen).

Ellison has always been interested in the properties of organic radicals (absolute heats of formation, ionization energies, electron affinities, and geometries). He continues to collaborate with the groups of John F. Stanton (University of Florida), Branko Ruscic (Active Thermochemical Tables, Argonne National Laboratory), Michael C. McCarthy (Harvard's Center for Astrophysics), Henry Kapteyn and Margaret Murnane (JILA).