

“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,
Eötvös University, Budapest, Hungary:

2000	Henry F. Schaefer III	2007	Mark Hoffmann
2001	Rodney J. Bartlett	2008	Hiroshi Nakatsuji
2002	John F. Stanton	2009	Enrico Clementi
2003	Josef Paldus	2010	Wilfried Meyer
2004	Debashis Mukherjee	2011	István Mayer
2005	Jürgen Gauss	2012	Hans Lischka
2006	Ingvar Lindgren		

13th ANNUAL
EDE KAPUY
MEMORIAL LECTURE

Thursday, 24th of May, 2012
4:30 P.M. auditory 062 (Gróh room),
Institute of Chemistry
Eötvös University
1117 Budapest, Pázmány sétány 1/A

Hans Lischka

**“Application of Multireference Theory:
From the Photodynamics of Nucleobases to
Graphene Multiradical Structures”**

Presented by the
Laboratory of Theoretical Chemistry
Eötvös 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.

HANS LISCHKA

was born in Vienna, Austria, in 1943. He studied Chemistry at the University of Vienna and finished his PhD (under the supervision of Prof. O. E. Polansky) in 1969 with a thesis on the parameterization of the Huckel method for UV spectra. In the years 1972 to 1973 he worked as a Humboldt Fellow with Professors Kutzelnigg and Ahlrichs at the University of Karlsruhe: he collaborated in the development of the “Karlsruhe CEPA program” and worked on the calculation of intermolecular forces under inclusion of electron correlation. In 1976 Hans Lischka completed his habilitation entitled “Ab initio calculations of intermolecular interactions with inclusion of electron correlation effects”. In 1980 he was visiting professor at the Ohio State University in Columbus/Ohio with a Max-Kade-Fellowship, where he started to develop the COLUMBUS program system in collaboration with I. Shavitt and R. Shepard. From 1976 to 1980 he was assistant professor at the Institute for Theoretical Chemistry of the University of Vienna and in 1980 he became professor of chemistry. He stayed several times as visiting scientist at the Argonne National Laboratory and the Pacific Northwest National Laboratory. In 1992-1996 Hans Lischka was the head of the Institute for Theoretical Chemistry and Radiation Chemistry of the University of Vienna, in the time of 2000-2004 and 2006-2008 he became vice-director of the Institute for Theoretical Chemistry and Structural Biology of the University of Vienna. In 1993-1995 he served as head of the Vienna section of the Austrian Chemical Society and in 2000-2001 as chairman of the Austrian Chemical Physical Society. He was a longtime member of the COST chemistry management committees and chairman of a COST Chemistry D37 Working Group “Computational Photochemistry and Photobiology”, and is founding member of the Managing Committee of the Central European Symposium for Theoretical Chemistry (former Triangular Symposium) and national coordinator until 2010.

In 2008 Hans Lischka retired from the University of Vienna and became visiting professor at the Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, from 2008-2010. In 2008 he was selected as first choice for a full professor position in Theoretical Chemistry at the Federal University of ABC, Sao Paulo, Brazil. In January 2011 he became senior research associate at the Texas Tech University in Lubbock, Texas, where he is research professor since September 2011.

Hans Lischka is author or co-author of more than 250 scientific publications and receives invitations to lectures at international conferences and at universities all over the world. His work was honored by the Sandoz Prize for Chemistry in 1980 and by two international symposia in 2003 and 2008 on the occasions of his 60th and 65th birthday, respectively. A special issue in Chemical Physics was dedicated to him to celebrate his 65th birthday.

He advised nine masters and twelve PhD students, as well as hosted fifteen postdoctoral scholars. Dr. Lischka is most known as the main developer of the COLUMBUS MRCI program system and NEWTON-X semi-classical molecular dynamics package. The latter is based on the analytic gradient capabilities of the former package, a unique feature in the world of MR-CI. The combination of these two programs enable scientists to locate conical intersections on the excited state energy surfaces and perform excited state dynamics. These capabilities are accelerated the understanding of the processes taking place in DNA after irradiation and opened up the possibility for several new applications on excited state.