“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**	**2012**	**Hans Lischka**
2001	**Rodney J. Bartlett**	**2013**	**Werner Kutzelnigg**
2002	**John F. Stanton**	**2014**	**Paul G. Mezey**
2003	**Josef Paldus**	**2015**	**Paul Ayers**
2004	**Debashis Mukherjee**	**2016**	**Trygve Ulf Helgaker**
2005	**Jürgen Gauss**	**2017**	**Jerzy Ciosłowski**
2006	**Ingvar Lindgren**	**2018**	**Jean-Paul Malrieu**
2007	**Mark Hoffmann**	**2019**	**Markus Reiher**
2008	**Hiroshi Nakatsuji**	**2021**	**Jozef Noga**
2009	**Enrico Clementi**	**2022**	**Barney Ellison**
2010	**Wilfried Meyer**	**2023**	**Gustavo Scuseria**
2011	**István Mayer**	**2024**	**Peter Knowles**

25th ANNUAL

EDE KAPUY MEMORIAL LECTURE

Thursday, 25th of September, 2025
15:00 P.M. auditory 063 (Bruckner Hall),
Institute of Chemistry
ELTE Eötvös Loránd University
1117 Budapest, Pázmány sétány 1/A

Martin Head-Gordon

Perturbation theory for electron correlation made better and faster?

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.

MARTIN HEAD-GORDON

Martin Head-Gordon completed B.Sc. (Hons) (1983) and M. Sc. (thesis) (1985) degrees at Monash University in Melbourne Australia, before coming to America to obtain his Ph. D. (1989) in theoretical chemistry at Carnegie-Mellon University, working with the late Sir John Pople on molecular orbital theory and algorithms. From 1989-1992 Head-Gordon was a postdoctoral fellow at AT&T Bell Laboratories, working with John Tully. He explored gas-surface energy exchange, and developed new models for non-adiabatic energy flow. Since 1992 Head-Gordon has been on the faculty of the Chemistry Department at the University of California Berkeley, where he holds the Kenneth S. Pitzer Distinguished Professorship (since 2012). He also holds an additional appointment as a Senior Faculty Scientist in the Chemical Sciences Division of Lawrence Berkeley National Laboratory.

Head-Gordon's research is primarily in molecular electronic structure theory. He is known for development of linear scaling quantum chemistry methods, for development of new density functionals, for advances in energy decomposition analysis, and for work on catalysis modeling. He is one of the driving forces behind the Q-Chem quantum chemistry program. Some of his studies in the field of pair functions and many-body perturbation theory directly relate to the work of the late Ede Kapuy.

Head-Gordon is a Fellow of the Royal Society (2019), a member of the National Academy of Sciences (2015), an American Chemical Society Fellow (2012), a member of the American Academy of Arts and Sciences (2011), and member of the International Academy of Quantum Molecular Sciences (2006). He is an Associate Editor of Molecular Physics and is the President of the World Association of Theoretical and Computational Chemists (WATOC). He has served as Program Chair and Chair of the ACS Division of Physical Chemistry (2009-2010).

Apart from his versatility in research topics, Head-Gordon is also a highly prolific scientist, with over 900 publications to his name. He is a well-respected research advisor, as evidenced by the extensive alumni list of his group. Among the more than 100 former members, many have become distinguished professors in the United States, Europe, and the Middle and Far East.