"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**		

24th ANNUAL

EDE KAPUY MEMORIAL LECTURE

Thursday, 14th of November, 2024
15:00 P.M. auditory 063 (Bruckner room),
Institute of Chemistry
ELTE Eötvös Loránd University
1117 Budapest, Pázmány sétány 1/A

Peter Knowles

How far can we go with single-configuration quantum chemistry?

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.

PETER KNOWLES

Peter Knowles was born on 4 March, 1960 in Liverpool, England. After undergraduate studies in Natural Sciences at Trinity College, Cambridge, he began a PhD in 1980 in the group of Nicholas Handy, developing algorithms for the multiconfigurational self-consistent field (MCSCF) method, including early implementation of the first and second nuclear gradients.

He was appointed as Research Fellow, St. Catharine's College in 1983, and in the following years made a number of contributions to quantum chemistry methodology: technology for full configuration interaction (FCI), algorithms for MCSCF and contracted multireference CI (with H.-J. Werner, starting the Molpro software package), perturbation theory for open-shell systems (with N. C. Handy and J. A. Pople). An important outcome of the availability of software for FCI was a numerical investigation of the convergence of many-body perturbation theory to high order, showing for the first time the very poor convergence in spin-contaminated description of open-shell states, and in molecules with low-lying excited states.

In 1985-86, he worked in the group of Bill Meath (Western Ontario, Canada) on the computation of non-covalent interactions between touching molecules, calculating for the first time explicitly the dispersion damping functions that are prevalent in many empirical force fields.

He has held academic positions at the University of Sussex (Lecturer, 1989-95), University of Birmingham (Professor, 1995-2004) and Cardiff University (Professor, 2004-2024).

As a complement to multireference methods, he has pursued the use of single reference configuration methods for use in strongly-correlated systems, establishing the characteristics of unitary, extended and variational coupled-cluster theories, leading to viable approximations to variational coupled cluster, and improved single-reference perturbation theory.

Recent work has included the extension of electronic many-body methods to systems with significant fermion-boson correlation, including beyond-Born-Oppenheimer quantum mechanics without potential energy surfaces, and the prediction of the properties of molecules in an optical cavity.

He has made a number of technical contributions to quantum chemistry methodology, specifically in quadrature of density functionals, and general parallel algorithms, and more generally through the development of the widely-used Molpro package.

Knowles' work has been recognised through the awards of the Royal Society of Chemistry (Harrison 1989, Marlow 1994, Computational Chemistry 2004), election as a Fellow of the Learned Society of Wales (2011), and election to membership of the International Academy of Quantum Molecular Sciences (2018).