“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**	**2013**	**Werner Kutzelnigg**
2001	**Rodney J. Bartlett**	**2014**	**Paul G. Mezey**
2002	**John F. Stanton**	**2015**	**Paul Ayers**
2003	**Josef Paldus**	**2016**	**Trygve Ulf Helgaker**
2004	**Debashis Mukherjee**	**2017**	**Jerzy Ciosłowski**
2005	**Jürgen Gauss**	**2018**	**Jean-Paul Malrieu**
2006	**Ingvar Lindgren**	**2019**	**Markus Reiher**
2007	**Mark Hoffmann**	**2021**	**Jozef Noga**
2008	**Hiroshi Nakatsuji**	**2022**	**Barney Ellison**
2009	**Enrico Clementi**	**2023**	**Gustavo Scuseria**
2010	**Wilfried Meyer**	**2024**	**Peter Knowles**
2011	**István Mayer**	**2025**	**Martin Head-Gordon**
2012	**Hans Lischka**		

26th ANNUAL

EDE KAPUY MEMORIAL LECTURE

Thursday, 5th of November, 2026
15:00 P.M. Richter room,
Institute of Chemistry
ELTE Eötvös Loránd University
1117 Budapest, Pázmány sétány 1/A

Leticia González

Light-Driven Chemistry through Molecular Simulation

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.

LETICIA GONZÁLEZ

Leticia González was born on 17 March, 1971 in Madrid (Spain). She graduated in Chemistry at the Universidad Autónoma de Madrid in 1994 and complemented her studies with a Master of Science in Chemistry at King's College London in 1995. She then returned to Madrid to pursue her doctoral studies, supported by a fellowship of the Spanish Ministry of Science, and obtained her PhD in Chemistry in 1998, distinguished with the Extraordinary Doctorate Award and later recognized as the Best PhD Thesis of her year at the Universidad Autónoma de Madrid.

In 1999, supported by an Alexander von Humboldt Fellowship, González moved to the Freie Universität Berlin, where she became C1 Assistant Professor and, in 2004, completed her Habilitation in Theoretical Chemistry. A Heisenberg Fellowship of the German Research Foundation followed in 2007, the same year she was appointed W2 Professor for Physical and Theoretical Chemistry at the Friedrich-Schiller-University of Jena. In 2011 she was called to the University of Vienna as Full Professor for Computational and Theoretical Chemistry, a position she still holds.

The main contribution of Leticia González to theoretical chemistry is the development of computational methods to unravel molecular reaction mechanisms driven by light. She has been a driving force in advancing computational photochemistry and ultrafast molecular science, devising original methods for excited-state dynamics, that describe non-adiabatic processes beyond the state of the art. She is the leading figure in the development of the molecular dynamics software named SHARC, standing for Surface Hopping including ARbitrary Couplings. SHARC was the first molecular dynamics package to incorporate spin-orbit coupling on the same footing as nonadiabatic coupling, together with a nonperturbative treatment of laser fields, opening a way to study e.g. electric field control of reaction barriers. The methodologies developed in her group led to successful applications on organic photoswitches, DNA building blocks and transition-metal photocatalysts, explaining and predicting how molecules behave when they absorb light or how can be controlled with shaped laser pulses.

González is author of more than 400 scientific publications and has delivered almost 300 invited lectures around the world, including numerous named Lectures. Her work has been recognized with the Dirac Medal of the World Association of Theoretical and Computational Chemists (2011), the Excellent Research Award of the Spanish Royal Society of Chemistry (2019), the Robert Bunsen Lecture Prize of the German Bunsen Society (2019) and the Doctor Honoris Causa of the Université de Lorraine (2018), among other recognitions. She is an elected Fellow of the European Academy of Sciences, a full member of the Austrian Academy of Sciences, a corresponding member of the Göttingen Academy of Sciences and Humanities, and an elected member of the International Academy of Quantum Molecular Sciences.

Beyond her research, González has taken on wide-ranging responsibilities within her institution and the international chemistry community. She currently serves in the Directorate of the Vienna Center for Advanced Studies and founded the Vienna Research Platform "Accelerating Photoreaction Discovery". She is Senior Editor at ACS Central Science and has served on the editorial and advisory boards of numerous journals including Angewandte Chemie, JACS Au and Chemical Science, and has long been an advocate for young researchers and for women in science.