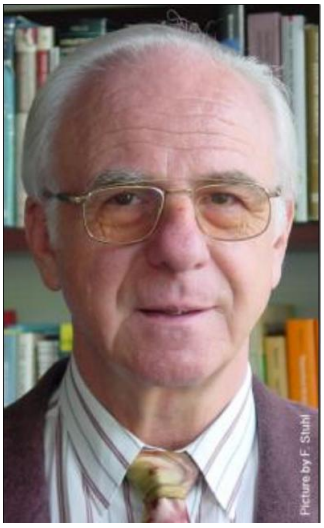
Werner Kutzelnigg, 1933–2019



Professor emeritus Dr. Werner Kutzelnigg, WATOC Fellow since 1995 and IAQMS Member since 1996, passed away on the 24th of November 2019 at the age of 86.

It is with great sadness that we learned of the passing away of Kutzelnigg. His work and leadership have played a seminal role in the development of the field of theoretical chemistry, in particular quantum chemistry, in Germany and worldwide, and he will be dearly missed.

Werner Kutzelnigg started his scientific career in theoretical chemistry in 1960, after completing his Ph.D. research in experimental molecular infrared spectroscopy. His early work on natural orbitals and, in particular, pair (or pseudo) natural orbitals (PNOs) has had a lasting impact on the treatment of the electron-correlation problem, which has always been at the heart of Kutzelnigg's work. Further significant contributions in this field have been his work on the unifying concept of "quantum chemistry in Fock space" and on the development of the R12 method to address the correlation cusp and the slow convergence of an expansion of the correlated wave function in orbital products. Work on the IGLO method (individual gauge for localized orbitals) has been an important contribution to the calculation of molecular properties, and Kutzelnigg has also made numerous important contributions to the field of relativistic quantum chemistry.

Werner Kutzelnigg was born on the 10th of September 1933 in Vienna, and his family moved to Germany in 1938. He studied chemistry at the Universities of Bonn and Freiburg i. Br. and received his Dr. rer. nat. (Ph.D.) with Reinhard Mecke in 1960. From 1960 to 1963 he was Postdoc with Bernard Pullman and Gaston Berthier in Paris, and from 1963 to 1964 with Per-Olov Löwdin in Uppsala. In 1967, he completed his habilitation on "*Die Behandlung des Mehrelektronenproblems der Quantenchemie durch unmittelbare Bestimmung der natürlichen Orbitale*" at the University of Göttingen. He was Associate Professor at the University of Karlsruhe (now Karlsruhe Institute of Technology, KIT) from 1970 to 1973 and Full Professor of Theoretical Chemistry at the Ruhr-University Bochum from 1973 until 1998, the year in which he was given emeritus status. He has published more than 250 scientific articles in journals of chemistry, physics and mathematics, and he has authored the textbook "*Einführung in die Theoretische Chemie*" (1975/1978), which has become a classic in teaching theoretical chemistry in Germany.

Kutzelnigg received several awards and prizes: the Carl Duisberg Memorial Prize of the GDCh (German Chemical Society) in 1971, the Schrödinger Medal of the World Association of Theoretical and Computational Chemists (WATOC) in 1995, and the Liebig Medal of the GDCh in 1996. He was elected to the International Academy of Quantum Molecular Science (IAQMS) in 1996. He received the Ilkovic Gold Medal of the Slovak Academy of Sciences in 1998, and he was the first awardee of the Erich Hückel Prize of the GDCh in 2016. Last summer, the Molecular Quantum Mechanics conference (MQM 2019) was held in Heidelberg in his honor, among others.

Wim Klopper, Karlsruhe, and Volker Staemmler, Bochum