

Reinhart Ahlrichs, 1940-2016



Professor emeritus Dr. Dr. h. c. Reinhart Ahlrichs, IAQMS member since 1992, passed away on the 12th of October 2016 at the age of 76. Ahlrichs has made important contributions to studies on the mathematical properties of Schrödinger operators, on the behavior of exact wave functions, and on the structure of intermolecular interactions. He has developed and applied various methods for molecular electronic-structure calculations. Work on the problem of electron correlation culminated in the coupled pair functional (CPF) approach. Under his directorship, the TURBOMOLE suite of programs was developed, which allows for the efficient *ab initio* treatment of properties such as energetics, structures, and spectra of electronic ground and excited states of large molecular systems with several 100 atoms – of all kinds. His most important driving force was to provide computational tools to tackle problems that originated from edge-cutting experimental chemistry. In the same way, his own applications to molecules were mainly carried out in connection with experiments to check, correct and to predict properties of molecules and their existence. Reinhart Ahlrichs was born on the 16th of January 1940 in Göttingen, Germany. He studied physics at the University of Göttingen (Diplom (M.Sc.) in 1965) and received his Dr. rer. nat. (PhD) in 1968 with Werner A. Bingel. From 1968-69 he was assistant in Göttingen with Werner Kutzelnigg and from 1969-70 he was postdoctoral fellow with Clemens C. J. Roothaan at the University of Chicago. From 1970-75 he was assistant at the Universität Karlsruhe (TH), now KIT Campus South, where he became Professor of Theoretical Chemistry in 1975. In addition to his professorship, he became Scientific Member of the Institute of Nanotechnology at Forschungszentrum Karlsruhe (now KIT Campus North) when the institute was founded in 1998. Professor Ahlrichs was given emeritus status in 2008. He has published ca. 300 scientific articles in journals of chemistry, physics and mathematics. In 1999, Ahlrichs received the Landesforschungspreis of the state Baden-Württemberg, and in 2000 he received the Bunsen Medal of the Bunsen Society for Physical Chemistry as well as the Liebig Memorial Medal of the Gesellschaft Deutscher Chemiker (GDCh). He was elected to the Heidelberg Academy of Sciences and Humanities in 1991, to the International Academy of Quantum Molecular Science in 1992, and to the Göttingen Academy of Sciences and Humanities in 2008. In 2015, Ahlrichs received an honorary doctorate from the Humboldt University in Berlin.