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chimica

Seminar

Prof. Dr. Henry F. Schaefer III

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Quantum Chemistry and Computer Science: A Historical Account of their Tightly Coupled Parallel Development

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Dipartimento di Chimica - *Aula Diagonale (I piano) ore 12*
Via Pietro Giuria 7, 10125 Torino

Prof. Dr. Henry F. Schaefer III is a computational and theoretical chemist who received a Ph.D. degree in chemical physics from Stanford University in 1969 where worked on ab initio electronic structure theory and quantum chemistry examining the electronic structure of first-row atoms.

He became an assistant professor of chemistry at the University of California, Berkeley in 1969 where he worked till 1987. In 1979-1980, he was appointed as the Wilfred T. Doherty Professor of Chemistry and inaugural Director of the Institute for Theoretical Chemistry at the University of Texas, Austin. In 1987, he moved to the University of Georgia where he is the Graham Perdue Professor of Chemistry and Director of the Center for Computational Chemistry.

During his career, he was visiting professor in various universities around the world and awarded with many prizes from the American Chemical Society, Royal Society of Chemistry, Alexander von Humboldt Foundation, to cite a few. He was also elected president of WATOC (World Association of Theoretical and Computational Chemists) in 1996, and held the position until 2005.

With the help of early IBM mainframes (as well as later supercomputers) he and his research group developed various computer-based methods for advanced quantum chemistry. Some of them include the multiconfiguration self-consistent-field (MCSCF), configuration interaction, coupled-cluster and Brueckner methods, and associated analytic gradient techniques.

Prof. Schaefer is one of the most prolific and highly cited chemists in the world, with more than 1,600 peer-reviewed publications and a Thomson Reuters H-Index of 119.

For further information see: https://en.wikipedia.org/wiki/Henry_F._Schaefer_III.

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