From Early Days of the Coupled Cluster Theory to its Role as a Predictive and Benchmark Instrument in Computational Chemistry

Miroslav Urban

Comenius University, Faculty of Natural Sciences, Department of Physical and Theoretical Chemistry, 84105 Bratislava, Slovakia

Some memories on the "Prague school" of quantum chemistry in the present J. Heyrovský Institute of Physical Chemistry will be presented. Here, Jiří Čížek's breakthrough papers on CPMET and principles of Coupled Cluster methods were born in the sixties of the last century. Steps leading to the most frequently used CCSD(T) method will be summarized. The progress in still wider applicability of CC methods is impressive and will be demonstrated by several interesting examples.