THEORETICAL METHODS FOR THE STUDY OF THE ELECTRONIC STRUCTURE OF MOLECULES

Nowadays the correct description of the electronic structure of molecules still remains a great challenge, particularly for systems of large chemical interest, such as molecules during bond breaking/formation, radicals, transition metal complexes, and electronically excited states. To get a thorough understanding of these complex systems, innovative theoretical methods are required. The theoretical chemistry group has developed new methods to efficiently couple quality and computational effort.

GOALS

The research aims at the development of new theoretical methods for the description of molecular systems, wherein the electronic structure cannot be describe with a single electronic configuration, their implementation within efficient computational codes, and their application towards the study of complex chemical problems. A large effort is devoted towards the development of "Multireference perturbation theory" methods which will be applied towards the description of electronic excited states, and the understanding of magnetic coupling in polynuclear complexes based on transition metals. Moreover, the group is active in the development of methods able to describe the electronic structure of molecules in chemical (local) terms.

INSTRUMENTS AND METHODS

Methods: formal development of theory in the field of quantum chemistry, implementation of computational codes by using the FORTRAN programming language, high level calculations on computer clusters.
Instruments: quad-core computer clusters for parallel calculation within Linux operating system.

MAIN SUBJECTS

Physical chemistry, Theoretical chemistry, Computational chemistry

RESEARCH GROUP

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