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Department of Physical and Macromolecular chemistry

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Department of Physical and Macromolecular Chemistry
invites you for a seminar and a professor lecture

Molecules in states with different spin multiplicity: Theoretical approaches and applications

Lecture hall CH 3, Faculty of Science, Hlavova 8, Praha 2

on October 25th, 2023 at 14:00

speaker: Doc. Mgr. Jiří Pittner, Dr.rer.nat., DSc.

Dept. of Theoretical Chemistry, J. Heyrovský Institute of Physical Chemistry of the CAS, v.v.i.



It is well known that properties of a molecule in its electronically excited state can be fundamentally different from the ground states ones. This fact is the basis of photochemistry and photophysics, which study reactions and properties of excited molecules, and it has many applications in both technology and material science, as well as in life sciences. For example, the ubiquitous oxygen molecule, which is a triplet in the ground state, has a highly reactive excited singlet state with cytotoxic effects. A photodynamic cancer therapy has been suggested, where a suitable photosensitizer molecule implanted in the tumor cell produces after photon absorption the singlet oxygen, which attacks the cell membrane. As an example, from material science we can mention the OLED displays, where the energetical efficiency could be greatly improved if a suitable molecule with the first excited triplet state lying energetically higher than the first excited singlet could be found.

Theoretical modeling and understanding of such phenomena require advanced methods of quantum chemistry. First of all, one has to be able to compute with sufficient accuracy the energies (and possibly also other properties) and understand the electronic structure of the states involved. Particularly challenging are molecules in the strongly correlated regime, i.e. with a small HOMO-LUMO gap, where several states are energetically close lying and more than one Slater determinant has a large weight in the wave function. We have developed multireference coupled cluster methods and coupled cluster methods externally corrected by the density matrix renormalization group, which are applicable in such situations. A brief overview of these developments will be presented, with most recent application to the cyclazine molecule, where the inverted singlet-triplet gap energetics is presently being debated in the literature.

Besides the "static" picture, where energies and time-independent properties of molecular states are investigated, the understanding of chemical processes often requires a time-dependent study. This can be performed employing molecular dynamics (MD), most often with (semi)classical treatment of the motion of atomic nuclei. When several excited states are included in the MD treatment in addition to the ground state, the method is called non-adiabatic molecular dynamics, and can be used to model photochemical processes like the internal conversion and the intersystem crossing. We have developed methods for computationally efficient non-adiabatic MD based on ADC(2) or TDDFT electronic structure treatment. Recently we investigated a halogen-derivative of the BODIPY molecule, which after a photoexcitation undergoes fast singlet-triplet transition and has thus the potential to serve as an efficient photosensitizer.

Organizers: Prof. Tomáš Obšil, Dr. Ondřej Sedláček

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