AB INITIO INVERSTAGATION OF THE EXCITED STATES OF NUCLEOBASES AND NUCLEOSIDES

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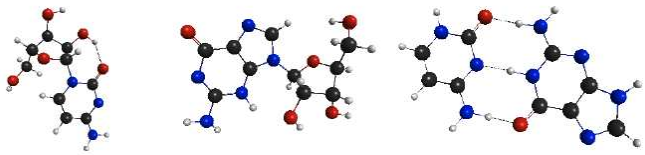

Most living bodies are exposed to sunlight, essential life sustaining processes are using this natural radiation. Sunlight has, however, several components (has a broad spectrum) and in particular the invisible component (UV, ultraviolet) is harmful for living organisms. Scientists around the word are busy to understand what happens in the cell when it is exposed to light: it seems that the building blocks of cells and in particular those carrying the genetic information (DNA and RNA) are highly protected against this exposition. Our research focuses on the spectral properties of the building blocks of DNA and RNA, the so called nucleobases and nucleosides, in order to understand this mechanism.

Due to improvement in computer technology both at hardware and software side we are now able to use the most accurate methods of *ab initio* quantum chemistry to investigate the spectroscopic properties of these building blocks. These calculations provide direct information on the properties of these molecules but also provide important benchmarks for cheaper methods which can be used for even larger systems.

We have calculated the excited state properties for the nucleobases (cytosine, guanine and adenine), their complexes with water and with each other (Watson-Crick base pairs and stacks) as well as corresponding nucleosides at the EOM-CCSD(T)/aug-cc-pVDZ level of theory and try to answer the following questions: (1) how the order of excited states varies in different nucleobases; (2) how hydration influences the excitation energy and order of excited states; (3) is there any effect of the sugar substituent; (4) how do close lying other bases change the spectrum. The calculations involve over hundred correlated electrons and up to thousand basis functions. Such calculations are now routinely available with the recently developed ACESIII code[a] and can make use of hundreds or even several thousand of processors.

[a] V. Lotrich, N. Flocke, M. Ponton, A. Yau, A. Perera, E. Deumens, R. J. Bartlett, *J.* Chem. Phys, **2008**, *1*28, 194104.