DNA strand breakage upon interaction with UV light

Computational study of the size- and sequence-dependence of DNA strand breakage upon photoionization

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In Short

- Radiation damage of short DNA strands upon photoionization
- Size- and sequence-dependence of ionization energies of DNA
- Hole-delocalization in charged DNA stacks

The interaction of UV radiation with living organisms can lead for instance to mutations within the genome. At photon energies above the ionization threshold (> 8 - 9 eV), DNA strand breaks become the dominant form of DNA radiation damage. However, the processes leading to such DNA strand breaks, in particular their dependence on the DNA sequence, are barely explored. This proposal is part of a DFG funded research grant (Interaction of Vacuum UV radiation (6 - 12 eV) with complex DNA targets), which aims at providing a detailed characterization of the excitation/ionization below and right above the ionization threshold of short DNA strands and the investigation of the resulting DNA strand breakage. In this DFG project, oligonucleotides with well-defined sequences up to about 20 nucleotides are studied both experimentally and theoretically to reveal the influence of DNA sequence and local environment on the vacuum ultra violet (VUV) photon-induced DNA strand breakage.

Here, we apply for computer time for the most expensive electronic structure calculations that need to be carried out in this project and for which our local resources are not sufficient. The main objectives of the suggested calculations are (1) verification of the assumptions underlying the experimental determination of ionization potentials of neutral DNA strands via gas-phase VUV photo ionization mass spectroscopy; (2) study of the size- and sequence-dependence of the ionization energies of short DNA oligonucleotides; and (3) determination of the hole-delocalization in, and stability of, charged DNA stacks.

To this end, we will run hybrid DFT and non-self-consistent G_0W_0 calculations for DNA oligonucleotides with well defined lengths and sequences. The calculations complement experiments which are currently carried out by collaborators. The goals is that the combination of theoretical and experimental results will allow us to gain far-reaching insight into the mechanisms that dominate DNA strand breakage following VUV photoionization.

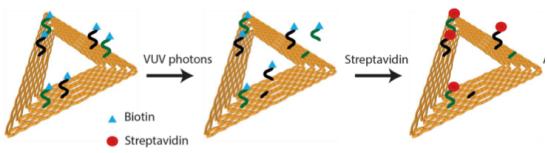

Figure 1: *Short DNA strands of well-defined length and sequence are fixed on DNA origami structures and irradiated with light. By marking the intact DNA strands, the number of strand breaks can be observed under the AFM.*

WWW

http://www.uni-potsdam.de/compchem

More Information

[1] L. Gallandi and T. Körzdörfer. J. Chem. Theory Comput., **11**, 5391 (2015).

doi:10.1021/acs.jctc.5b00820

[2] A. Keller, J. Rackwitz, E. Cauet, J. Liévin, T. Körzdörfer, A. Rotaru, K. V. Gothelf, F. Besenbacher, and I. Bald, Scientific Reports, **4**, 7391 (2014).

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Project Partners

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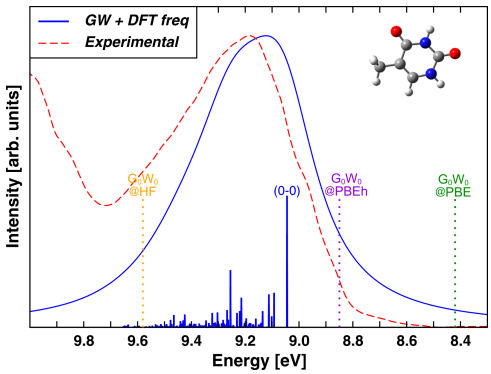

Figure 2: *The combination of density functional theory with G_0W_0 calculations allows us to determine the ionization energies of DNA nucleobases as well as short DNA strands from first principles with high accuracy.*