Supramolecular Quantum Chemistry: From DNA Base Pairs *via* Nanoswitches to Remote Communication

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Structure, bonding and reactivity are central issues, if not the core business, of chemistry. Yet, our understanding of chemical reactivity lags behind the minute understanding that we have today of covalent molecular structure and stability. But also our understanding of chemical bonding still shows gaps, for example, when it comes to weak interactions featuring in supramolecular chemistry, such as, hydrogen bonds and halogen bonds. I will address the nature, *i.e.*, the bonding mechanism, of hydrogen bonds and show that they have a sizable orbital-interaction component [1,2].
I will show that this covalent nature of hydrogen bonds can be exploited in rational design of supramolecular switches. My quantum chemical computations and analyses will reveal how the geometric shape and hydrogen bond strength of a modified DNA base pair can be chemically switched between 3 states, simply by protonation/deprotonation of substituents Y (see Figure 1). The origin of this switching is traced to the nature of the hydrogen bonding mechanism [3]. Interestingly, the proposed DNA-bases nanoswitches can be accessed remotely through the use of π-conjugated "organic wires" (see Figure 1) [4].

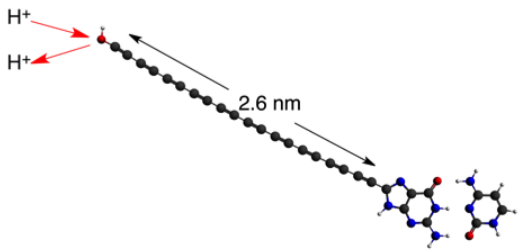

Figure 1: Remotely accessed supramolecular switch based on DNA.

I will also address methodological aspects (in particular, concepts and bond-analysis tools [5]) of our quantum chemistry software package, the Amsterdam Density Functional (ADF) program [6].

References

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