New Tools for the Analysis of Electronic Excitation Processes

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Owing to a tremendous effort in method development and to the availability of supercomputers it is possible nowadays to perform highly accurate simulations of complex excited state phenomena even in large systems. However, the wavefunctions produced in these computations are difficult to interpret if many interacting configurations and orbitals are involved. Even more, for large systems excitonic effects come into play, which are difficult to comprehend in a standard molecular orbital picture. Therefore, new analysis methods are direly needed to get full insight into the computations performed.

This talk will provide an overview over our recently developed wavefunction analysis framework,[1-3] which provides detailed visual and quantitative analysis tools for excited state computations. The power of these methods will be illustrated in three examples. First, a recent study on the absorbing states in single-stranded DNA will be presented.[4] In this case a rigorous and automated quantitative analysis is particularly beneficial when combined with structural sampling in this flexible multichromophoric system. Second, it will be discussed how the same analysis strategy can be extended to the case of transition metal complexes[5] and recent results on a Rhenium complex will be presented. Finally, the emergence of excitonic effects will be discussed in the case of conjugated polymers.[6] It will be shown that the exciton size in these systems scales uniformly with the system size and is independent of the molecular details. The description of these excitonic effects within time-dependent density functional theory will be discussed.

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