Light-induced electronic structure reorganization Topological insights

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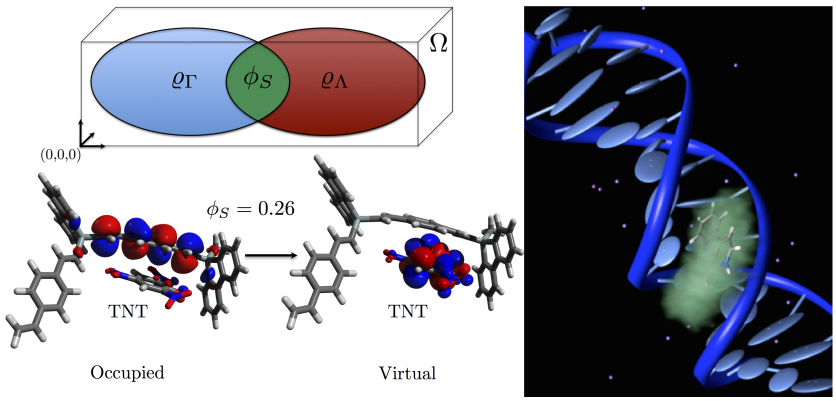
This contribution aims at providing a theoretical insight into the physical nature of chromophores' excited states with a method designed for quantitatively assessing the charge-transfer character of a given electronic transition. This new strategy allows to investigate the topology of the target excited states using the Detachment/Attachment Density Matrices and/or Natural Transition Orbitals methodologies. Those methods will be shown to be involved in the theoretical elaboration of the dimensionless ϕ_S quantum-chemical index, defined as the normalized spatial overlap between Detachment and Attachment densities in the direct space. This descriptor will also be introduced as an accurate diagnostic tool for exchange-correlation functionals in the framework of Time-Dependent Density Functional Theory. Afterwards, another topological descriptor will be used together with ϕ_S for deriving a general index which formally gathers the physical information coming from atomic and Euclidean spaces. The substitution of numerical integration by linear algebra for the evaluation of these indices will be introduced, and some applications of the ϕ_S descriptor will be presented in the scope of anti-cancer phototherapeutic agents, dye-sensitized solar cells and explosive probes design.



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References:

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