Insights into the Topology of Molecular Electronic Transitions
Theoretical Strategies

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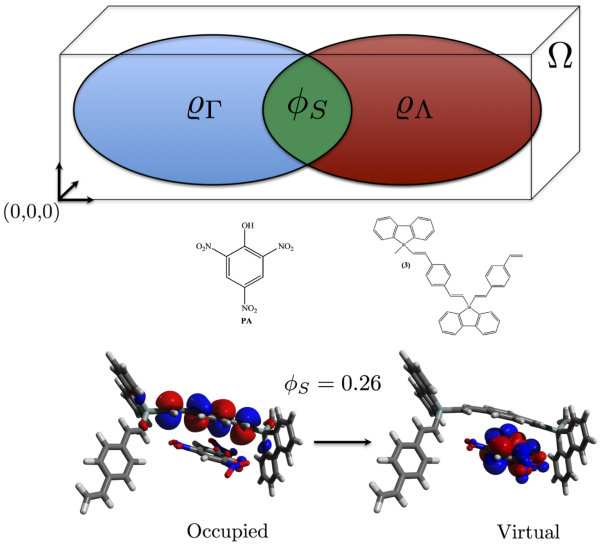
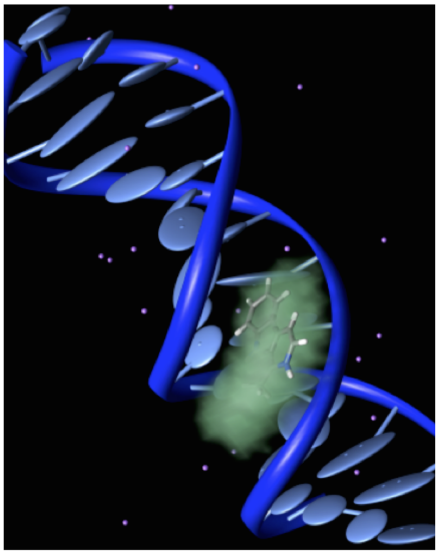
This talk aims at providing an insight into the physical nature of molecular excited states through the development of a quantitative method designed for numerically assessing the charge-transfer character of a given electronic transition. This new method allows us to investigate the topology of the target excited states according to Detachment/Attachment Density Matrices and/or Natural Transition Orbitals strategies. Those methodologies will be detailed, as they are involved in the theoretical elaboration of the ϕ_S quantum-chemical descriptor. The latter will also be introduced as an efficient diagnostic tool for exchange-correlation functional in the framework of Time-Dependent Density Functional Theory. Afterwards, a formerly developed topological descriptor will be combined to ϕ_S for deriving a general index gathering the physical informations coming from Hilbert and Direct space operations. The possibility of using linear algebra rather than numerical integration for the evaluation of these descriptors will be exposed, and some applications of the ϕ_S index will be presented in the scope of anti-cancer phototherapeutic agents, dye-sensitized solar cells and explosive probes design. MD-QM/MM post-processing perspectives will also be exposed.





1. Etienne, T. ; Assfeld, X. ; Monari, A. *J. Chem. Theory Comput.* **2014** *10*, 3896–3905 & 3906–3914.
2. Etienne, T. *J. Chem. Theory Comput.* **2015** *11*, 1692–1699.