Density based methods and descriptors for the modelling of molecular devices

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Theoretical tools enabling the description and the prediction of excited states' properties and reactivity are increasingly appealing for the rational design of new compounds and for the understanding and the optimization of the existing ones.

Ideally, these methods should both correctly reproduce the potential energy surfaces (PES) of the excited states, within and far from the Franck Condon region, and deliver a coherent picture of all photochemical processes occurring. Due to intrinsic complexity of the electronic excited states, this task is very hard for any quantum method especially when dealing with chemically relevant systems in realistic conditions.

To this end, in the last years, we introduced some strategies for the description of excited states, coupling Time-Dependent density functional theory (TD-DFT) with descriptors based on electron density. This type of indexes was primarily aiming at the diagnostic and description of excited states with a charge-transfer character, but recently extended to provide a qualitative identification of decay channels (both radiative or non-radiative).[1-8]

In this talk we will give an overview of these approaches –also coupled with embedding techniques for the description of the environment- and of their application to molecule-based devices.

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