Photoswitches Isomerization in Plasmonic Backgrounds

Master

Photoswitches are interesting molecules able to reversible switch between two or more isomers under a proper light illumination. Upon photo-irradiation, molecular photoswitches instantaneously modulate various physical and chemical properties of materials as well as biological functions, this making them chemical objects extremely promising for a post-synthesis control and/or tuning of photochemical properties.

Strong coupling of molecular excitations with surface plasmons or other localized photonic modes can favor the creation of hybrid half-light half-matter modes (i.e. polaritons) and lead to important energy shifts in such quantum systems with respect to the original uncoupled transition energies. The theoretical study of the polaritonic potential energy surfaces (poPES) can, thus, predict significant changes in the photoswitch behaviour under light-illumination, this opening the possibility to manipulate and control photochemical reactions in plasmonic backgrounds.

The Chair of Materials Science and Nanotechnology is looking for a highly motivated Master student able to perform a computational analysis within the framework of *Density Functional Theory* (DFT) and of its *Time-Dependent* extension (TD-DFT) of the potential energy surface (PES) curves of the groundstate and of the first excited states for a molecular switch of practical interest interacting with metallic nanoclusters.

The thesis would, thus, deal with concepts proper of *polaritonic chemistry*, a recent research field with a huge plethora of technological applications, going from drug discovery to photopharmacology.

The **research plan** will include:

1. Get familiar with DFT and TD-DFT frameworks.
2. Understand the basic principles of non-adiabatic coupling in photoswitches.
3. Compute PES curves within Quantum Espresso Package.
4. Learning HCP facilities use.

References

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- J. Fregoni, G. Granucci, M. Persico and S. Corni, Chem 6, 250-265 (2020).
- T. R. Nelson at al., *Chem. Rev.*, 120, 4, 2215−2287 (2020).