Modeling Photo-Responsive systems using combined classical and DFT approaches

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Photo-responsive materials are gaining ever-increasing attention thanks to their fast -- and often dramatic -- response and the relatively non-invasive nature of light as a stimulus [1].
Nonetheless, understanding the excited state mechanisms that are at the basis of these materials is very challenging both for theory and for experiments. If indeed ground state properties of condensed systems (ex. crystalline or amorphous phases) are currently feasible and even if excited states description has greatly advanced [2,3,4] this latter is often associated with nontrivial computational expense so that the study of excited state reactivity, mechanochromism, piezochromism, heterogeneous photocatalysis, and photoemission, remains a significant challenge for theoretical approaches.
In this talk, we present the contribution of our group to the modeling of some of these phenomena, combining different theoretical tools ranging from classical to quantum approaches in either molecular or periodic formalisms [5-7]. We demonstrate that by choosing, developing and combining suitable theoretical tools, such phenomena can be qualitatively (or even quantitatively) described.

References

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