Optical excitations in organic semiconductors: What do we learn from *ab initio* many-body theory?

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The research on organic semiconductors has significantly benefited in the last decade from the advancement of *ab initio* many-body theoretical methods, that enable parameter-free description and deep understanding of the electronic and optical properties of these materials. In this talk I will illustrate the ability of density-functional theory and many-body perturbation theory to shed light into the nature of optical excitations in different types of organic semiconductors, ranging from crystalline pentacene polymorphs [1], to J-aggregates of push-pull molecules [2], to donor/acceptor complexes [3-5]. After a brief review about the theory, I will demonstrate the predictive power of this approach and discuss its challenges in view of a meaningful connection to experiments.

References

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