Insight on excitons in organic and hybrid materials from first-principles many-body theory

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The diversified nature of quasiparticles that are generated in materials upon their interaction with light calls for an in-depth understanding that can be efficiently and reliably provided by *ab initio* methods. Density-functional theory and many-body perturbation theory are the state-of-the-art approaches to tackle these challenges. In this colloquium, I will briefly review these methods and, with the aid of a few significant examples, I will demonstrate their ability to disclose the nature of excitons in a variety of materials, ranging from organic semiconductors [1-3] even in their crystalline arrangement [4-6], to hybrid organic/inorganic interfaces [7,8]. I will also discuss how the gained insight can be straightforwardly connected with experimental observations, in order to achieve a comprehensive knowledge of such complex systems.

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