

QED materials engineering: first principles modeling of polaritonic matter

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We provide an overview of how well-established concepts in the fields of quantum chemistry and materials have to be adapted when the quantum nature of light becomes important. We will pursue the question whether it is possible to create these new states of materials as groundstates of the system. To this end we will show how the emerging (vacuum) dressed states resembles Floquet states in driven systems. A particular appeal of light dressing is the possibility to engineer symmetry breaking which can lead to novel properties of materials. Strong light-matter coupling in cavities provides a pathway to break fundamental materials symmetries, like time-reversal symmetry in chiral cavities. We will discuss the potential to realize non-equilibrium states of matter that have so far been only accessible in ultrafast and ultrastrong laser-driven materials. We illustrate the realisation of those ideas in molecular complexes and 2D materials and show that the combination of cavity-QED and 2D twisted van der Waals heterostructures provides a novel and unique platform for the seamless realisation of a plethora of interacting quantum phenomena, including exotic and elusive correlated and topological phases of matter. We will briefly introduce our newly developed quantum electrodynamics density-functional formalism (QEDFT) as a first principles framework to predict, characterize and control the spontaneous appearance of ordered phases of strongly interacting light-matter hybrids.