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Strong light matter phenomena in molecules and low dimensional systems: from first principles

Content

Strong-field effects and time-resolved spectroscopy can be used to expose dynamical, structural, and electronic properties of molecules. Here we present work that investigates these effects with different flavors of first-principles calculations. We will 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 ground states 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 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.

Primary author: Prof. RUBIO, Angel (MPSD (Max-Planck-Forschungsgruppe))

Presenter: Prof. RUBIO, Angel (MPSD (Max-Planck-Forschungsgruppe))

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