Ab initio cavity quantum electrodynamics

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Strong coupling of photonic and molecular degrees of freedom can lead to the formation of hybrid light-matter states known as polaritons whose properties can be dramatically different than those of the original uncoupled species. The unique properties of these states have inspired the development of a variety of theoretical and computational tools with the hope that they can facilitate light-mediated control over materials properties or chemical transformations. In particular, several ab initio cavity quantum electrodynamics (QED) theories have recently emerged as a powerful approaches for the description of polariton states in molecular systems. I will discuss QED generalizations of several well-known quantum chemical methods and their application to to cavity-bound molecular systems.