Relativistic polaritonic chemistry : a wave-function based ab initio perspective

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Recently, new experiments based on superconducting cavities have been designed to couple electronic spins of single-molecule-magnets with the magnetic component of a quantum electromagnetic field [1]. As a result, this opens a door to new technological applications (e.g. quantum computing). In these experiments, the matter states strongly couple with quantum states of the electromagnetic field, generating hybrid states known as polariton with mixed light and matter character. This is part of a larger and emergent field of research known as polaritonic chemistry [2].

In spite of the growing attention dedicated to the latter in the last decade, the fundamental physics underlying these phenomena and their impact on the chemical properties of molecular systems is still unclear. In order to shine some lights on the mechanisms at play, many theoretical approaches have been designed. In particular, several ab initio quantum chemistry methods (DFT, CC, CI, etc.) have been extended to investigate molecular systems in strong light-matter coupling conditions [3,4].

In this seminar, we will present a new Relativistic Hartree-Fock theory for coupled electron-photon systems [5]. Indeed, the inclusion of relativistic effects becomes crucial if heavy elements are present in the system and more generally if magnetic properties need to be investigated. During the talk, the proposed methodology will be explained and its application to small molecular systems containing heavy atom will be presented. Particular attention will be devoted to the analysis of the competition between relativistic and field induced effects.

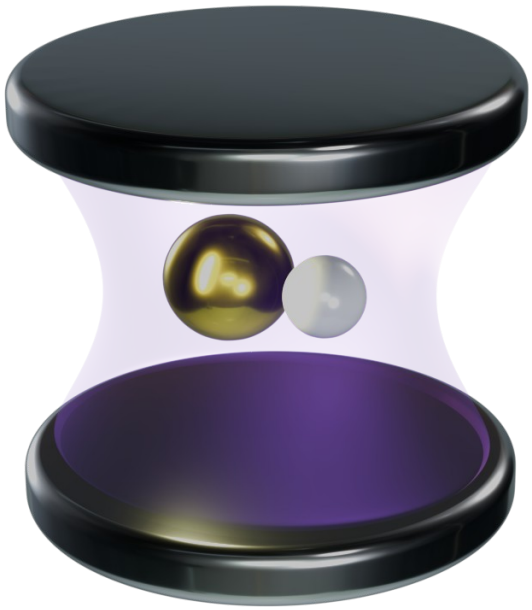

Figure 1: Schematic representation of an optical cavity

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