Università degli Studi di Messina
Dottorato di Ricerca in Fisica

# Appunti di Fisica '20
# &
# Dottorato di Ricerca in Fisica

**17 dicembre ore 15:30**

webinar su Microsoft Teams

## Changing ground state molecular properties in optical cavities: an *ab-initio* study

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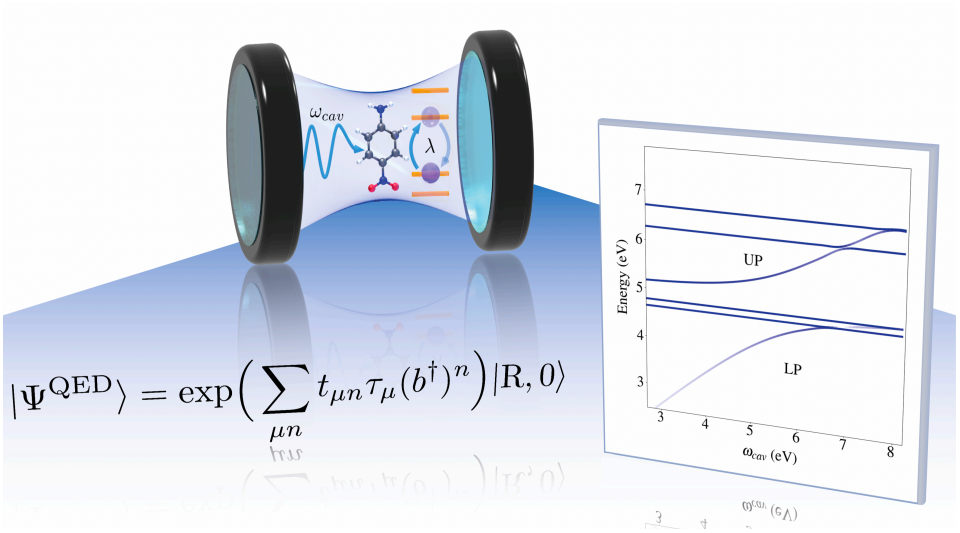
Manipulation of matter properties using strong coupling to photons is becoming a hot research topic in physics and chemistry [1,2]. Recent experimental studies demonstrated that strong-light matter coupling in optical cavities can be used to inhibit, catalyze and increment the selectivity of chemical reactions.

In the past few years, a lot of progress has been made in the field, but a complete understanding of the possibilities offered by cavity QED in chemistry is still far from being achieved.

In quantum optics, strong light-matter interaction has been extensively investigated since the 1950s using model Hamiltonians and a broad range of fascinating insights has been accessed. However, these approaches are not quantitative. For instance they typically cannot predict changes in the molecular ground state.

In this talk, I will present some recent *ab-initio* theoretical studies we performed on chemical systems. Quantum electrodynamics coupled-cluster (QED-CC) [3], configuration interaction (QED- FCI) [4] and density functional (QEDFT) [2] approaches have been applied. We have demonstrated that molecular ground states can be modified by optical cavities. Considering the size of the effects, we are convinced that our predictions can be observed experimentally. In the last part of the talk, I will show some interesting perspective applications of this fascinating field.




[1] T. W. Ebbesen, Acc. Chem. Res., **49**, 2403 (2016)
[2] M. Ruggenthaler, N. Tancogne-Dejean, J. Flick, H. Appel, and A. Rubio, Nature Rev. Chem., **2**, 0118 (2018)
[3] T. S. Haugland, E. Ronca, E. F. Kjønstad, A. Rubio and H. Koch, arXiv, **2005.04477**, 2020 (**Accepted in Physical Review X**)
[4] T. S. Haugland, C. Schäfer, E. Ronca, A. Rubio and H. Koch, **soon on ArXiv**.

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