CAVITY-CONTROLLED CHEMISTRY BY TIME-DEPENDENT DENSITY FUNCTIONAL THEORY

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : iLM

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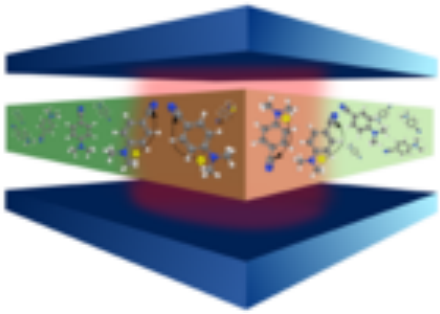
CONTACT(S) : NIEHAUS Thomas

CONTACT(S) DETAILS: thomas.niehaus[at]univ-lyon1.fr / Tel. 0472431571

KEYWORD(S) : Polaritons / TDDFT / Cavity

SCIENTIFIC CONTEXT :



Confining the electric field in cavities can lead to ultra-strong light-matter interaction. This allows to control the excited state dynamics of molecules in unprecedented ways. The luminescence properties are strongly modified and also chemical reactions might be taylored by appropriate cavity fields [1]. In recent years excited state phenomena of nanostructures and molecules were successfully treated at the level of time-dependent density functional theory (TDDFT). This theory solves the time-dependent Schroedinger equation for many-electron systems based on an exact formalism for the electron density. The electric field is treated classically and enters through the dipole approximation. In order to describe the light-matter interaction in cavities one needs to quantize the electric field and treat matter and fields at the same footing. The combined theory (QE-DFT) was only recently developed [2] and holds promise to describe cavity-controlled chemistry ab-initio without any empirical parameters.

MISSIONS :

In this thesis, we will implement and develop QE-DFT for the numerically highly efficient TD-DFTB method [3]. The conventional TD-DFTB method will be extended to include the coupling to cavity modes and will give rise to the description of correlated matter-field states, the polaritons. The implementation is done in the open-source code DFTB+ [4,5,6], a modern Fortran code that is run on high-performance computers by a large number of groups world wide. This thesis offers the unique possibility to work on cutting edge research and participate in the joint software development of an actively maintained project.

Some coding experience is required (not necessarily in Fortran).

OUTLOOKS :

This topic can be continued as PhD thesis.

BIBLIOGRAPHY :

[1] https://doi.org/10.1002/anie.201107033
[2] https://doi.org/10.1021/acsphotonics.9b00768
[3] https://doi.org/10.1016/j.theochem.2009.04.034
[4] https://doi.org/10.1063/1.5143190
[5] https://dftbplus.org/
[6] https://github.com/dftbplus/dftbplus

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