DYNAMICS OF ORBITAL MAGNETISM IN SYMMETRIC MOLECULES

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : Institut Lumière Matière (iLM)

LEVEL : M1 / M2
TEAM(S) : THEOCHEM

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KEYWORD(S) : Real-Time (RT) TDDFT / Inverse Faraday Effect / Clusters

SCIENTIFIC CONTEXT :

The collective nature of electron density oscillation at plasmonic excitations correspond to strong absorption of light energy at nanometric length scales. In nano-objects, especially in clusters of metals this energy can be localized around the surface of the clusters to give rise to localized surface-plasmon resonances (LSPRs). It has been shown that by modulating the polarization of the external perturbing electric field of light one can create orbital current at LSPR in metal nanoparticles (NPs) and clusters which in turn gives rise to magnetization [1, 2, 3] thanks to the Inverse Faraday effect (IFE). This light-field-induced orbital magnetism can be used to tune the opto-magnetic and/or magneto-optic properties even if the NPs are not intrinsically magnetic. For this very reason they are interesting for applications in nanophotonics devices [4] as corroborated by recent experimental works which reported quantification of optically induced magnetization in solution of plasmonic gold nanoparticles [1] but also in graphene [5] and gold [6] nano-disks. These studies have been focused to understand the fundamental working principles of orbital magnetism in plasmonic clusters of metals. To this end, this master thesis intends to address ab-initio theoretical exploration of light-induced orbital magnetism in clusters of non-metallic elements, and in organic molecular compounds.

MISSIONS :

The goal of this master internship is to theoretically investigate quantum many-body effects in the generation of orbital magnetic moments in large molecules like C60 , clusters of atoms, and/or metasurfaces using electromagnetic perturbation. Time-evolution approach of TDDFT will be employed to
perform ab-initio simulation of the interaction of electromagnetic field (which will be described classically) and periodic arrangement of metal clusters described using jellium spheres. After getting an introduction to the working principles of both static and time-dependent (TD) density-functional theory (DFT) the candidate will gain experience in performing ab-initio calculations using open-source codes (octopus and salmon). The simulations will be carried out on supercomputers in local and national centres.

REQUIREMENTS: An interest in numerical methods, programming in C++/Fortran and Python, high-performance computation using supercomputers, as well as knowledge of quantum mechanics are strongly solicited.

OUTLOOKS :

Possibility to apply for PhD.

BIBLIOGRAPHY :

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[4] J. Qin et al., Nanophotonics, 11(11):2639-2659, 2022.
[5] Jeong Woo Han et al., Nature Communications, 14(1):7493, Nov 2023.
[6] S. Parchenko et al., Adv. Photonics Res. 2025, 6, 2400083 .

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