LIGHT-INDUCED ORBITAL MAGNETISM

LABORATORY : Institut Lumière Matière

LEVEL : M1 / M2
TEAM(S) : THEOCHEM

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KEYWORD(S) : Clusters / Inverse Faraday Effect / TDDFT

SCIENTIFIC CONTEXT :

The delocalization of electron density is crucial for many observable light-matter interactions. For example, at nanometric length scales, it gives rise to collective oscillation of electron-density known as plasmon. In molecules, the delocalization of π electrons is a crucial aspect of aromaticity. It has been shown [1] that by using elliptically polarized laser field at plasmon energy one can create orbital current that corresponds to rotational motion of delocalized electrons in metal nanoparticles (NPs) and clusters [2, 3]. This rotating current in turn gives rise to magnetization thanks to the Inverse Faraday effect (IFE) even if the NPs are not intrinsically magnetic [1, 4]. Several recent studies [4, 5], therefore, have been focused to understand the fundamental working principles of this light-induced orbital magnetism. While the proof-of-concept results are already available for NPs, minute understanding of the quantum effects that influence this light-induced magnetism is primordial for harvesting it at quantum sizes, i.e., in clusters and molecules. To this end, both theoretical and experimental endeavors are strongly in motion.

MISSIONS :

In this master thesis, the objective is to theoretically investigate quantum many-body effects in the generation of orbital magnetic moments in large molecules, clusters of atoms, and/or metasurfaces of clusters 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 the system under study. 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. The long-term objective is to propose a new method for harvesting light-induced magnetism in metal nano-clusters and molecules that can be measured by experimental collaborator Mathieu Mivelle in INSP Paris.

REQUIREMENTS: An interest in high-performance computation using supercomputers, numerical methods, programming in C++/Fortran and Python, as well as in quantum light-matter interaction at nano-scale are strongly solicited.

OUTLOOKS :

Possibility (for M2 candidates) to apply for PhD .

BIBLIOGRAPHY :

[1] O. H.-C. Cheng et al., Nature Photonics, 14(6):365–368, Jun 2020.
[2] R. Sinha-Roy et al., ACS Photonics, 7(9):2429-2439, Sep 2020.
[3] Deru Lian et al., Nanophotonics, 13(23):4291-4302, 2024.
[4] Jeong Woo Han et al., Nature Communications, 14(1):7493, Nov 2023.
[5] S. Parchenko et al., Adv. Photonics Res. 2025, 6, 2400083 .

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