TIME-DEPENDENT DENSITY FUNCTIONAL THEORY SIMULATIONS FOR ATTOSECOND MOLECULAR DYNAMICS

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : iLM

LEVEL : M1 / M2
TEAM(S) : THEOCHEM

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KEYWORD(S) : TDDFT / Attosecond science / Molecular Physics

SCIENTIFIC CONTEXT :

The advent of attosecond physics has made it possible to observe and manipulate dynamic processes occurring on the intrinsic timescale of charge motion in atoms and molecules. This breakthrough has opened the door to realizing the long-standing dream of attochemistry—controlling chemical reactions by manipulating pure electron dynamics in the initial moments after system excitation. Recent advances, such as the demonstration of long-lived electronic coherences and the ability to alter a molecule's stability through pure electron dynamics, have made this an exciting time for the field. However, a current bottleneck in the realization of attochemistry is the ability to effectively trigger the desired pure electron dynamics via molecular photoionization.

MISSIONS :

In this project, we propose to study the photoionization of molecules exposed to ultrashort laser pulses. Simulating the ionization process poses a significant theoretical challenge due to the need to model a continuum. In this context, Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) in its real-space formulation offers a highly promising approach. The real-space formulation allows for a straightforward definition of ionization based on the simulation box. It also enables the calculation of experimental observables, such as the photoelectron spectrum, facilitating direct comparison between theory and experiment.

Recent studies have shown that ultrafast pure electron dynamics can be triggered through infrared multi-photon ionization using RT-TDDFT. This finding marks an important step in demonstrating the potential of RT-TDDFT in attosecond molecular physics. During this internship, we will systematically test the applicability and robustness of RT-TDDFT by simulating the ultrafast dynamics of molecular systems.

OUTLOOKS :

The internship may be followed by a PhD, subject to the availability of sufficient funding.

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