



LCT

Laboratoire de Chimie Théorique



Theoretical linear and non-linear optical spectroscopy in atoms, molecules and solids

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(Pôle 1 : Méthodes pour la chimie quantique)

Sorbonne Université

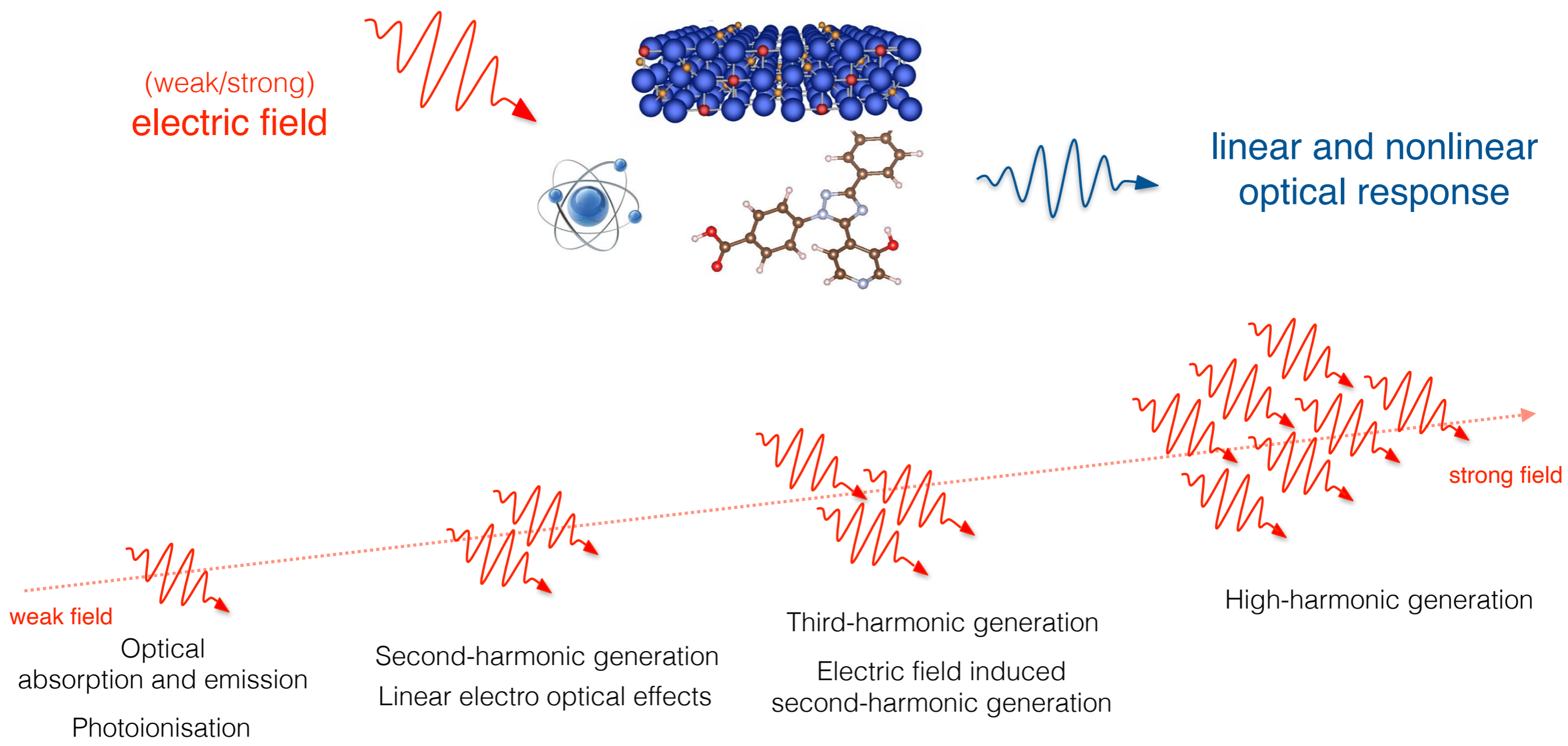
Journée UFR de Chimie / UFR de Physique

Quantum Chemistry methods

theory development

implementation in numerical codes

applications to real systems



Quantum Chemistry

accurate description of
many-electron systems



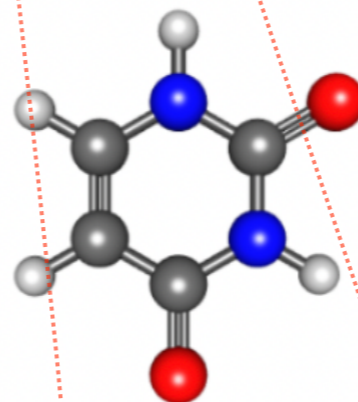
Strong field physics

High-Harmonic Generation
electron dynamics and molecular structure
attosecond pulses

continuum

ionisation

recombination



Morassut, Coccia, Luppi JCP (2023)

Toulouse, Schwinn, Zapata, Levitt, Cancès, Luppi JCP 2022

Coccia, Luppi J. Phys. Condens. Matter (2021)

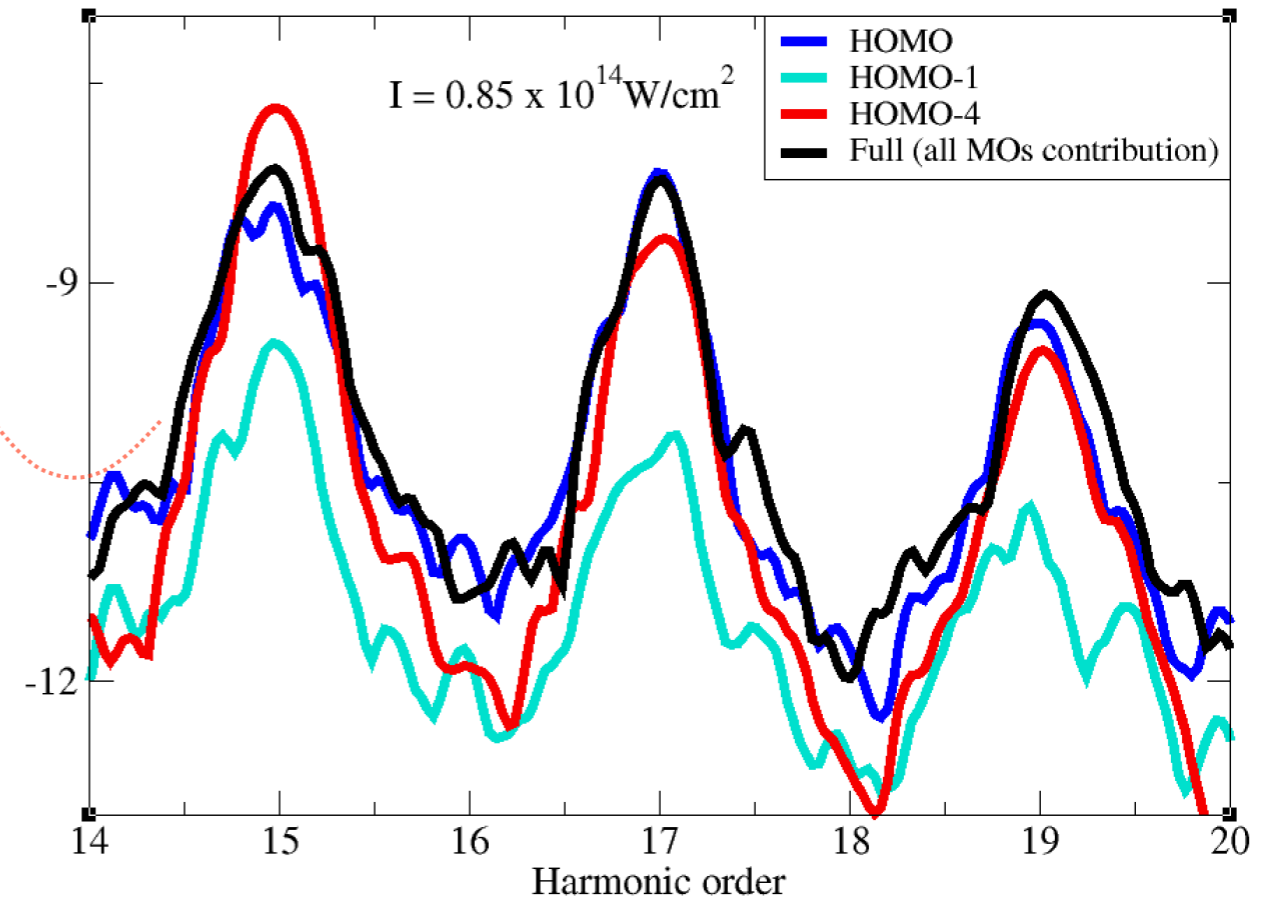
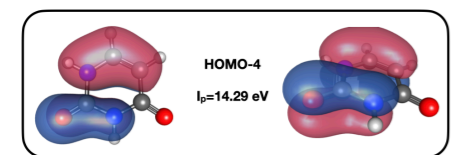
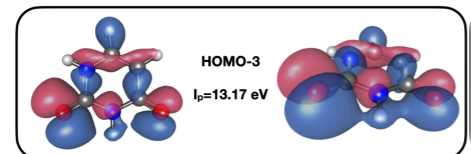
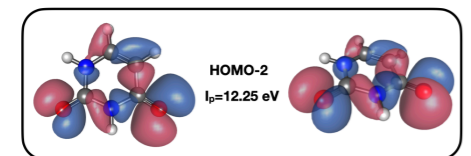
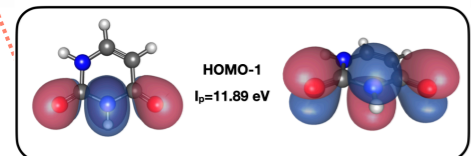
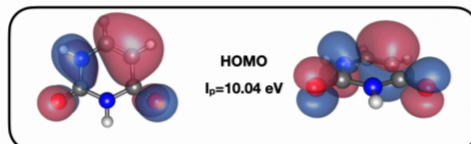
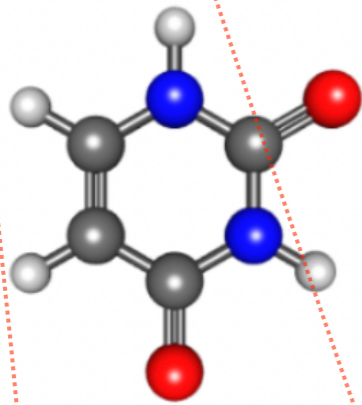
Luppi, Head-Gordon JCP (2013)

High-harmonic generation of uracil molecule

Role of the molecular orbitals as different channels of ionisation and recombination : symmetry versus energy

ionisation

recombination



Poster : Computation of High Harmonic Generation of molecules using Quantum Chemistry approaches

Thanks for your attention !