Master thesis projects

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Dipartimento di Scienze Chimiche e Farmaceutiche

Theoretical modelling of plasmon-assisted photocatalysis

Collaboration with Università di Padova
one PhD student (Leonardo Biancorosso)

Theoretical modelling of plasmon-assisted photocatalysis

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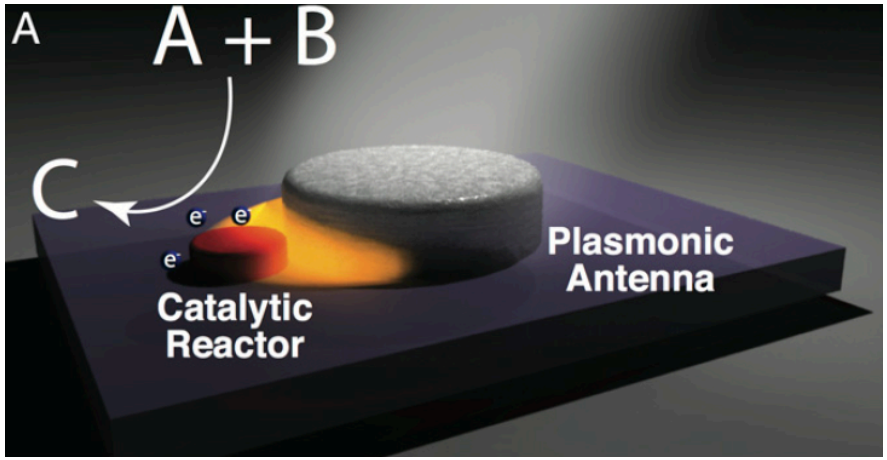
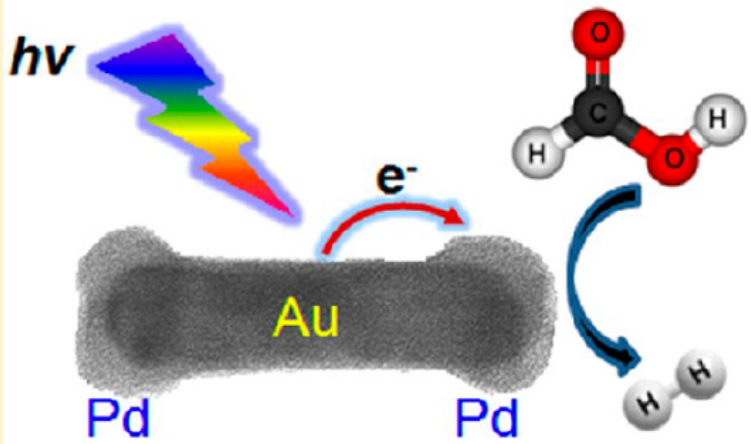
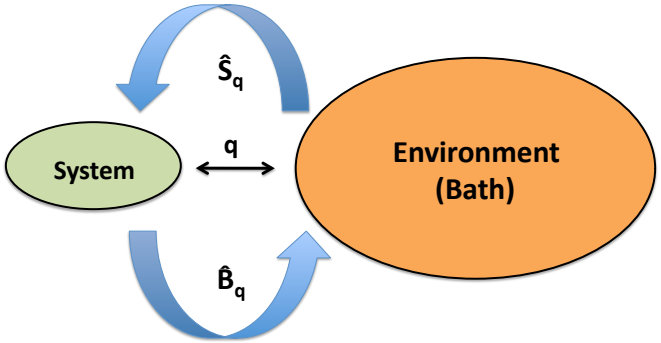
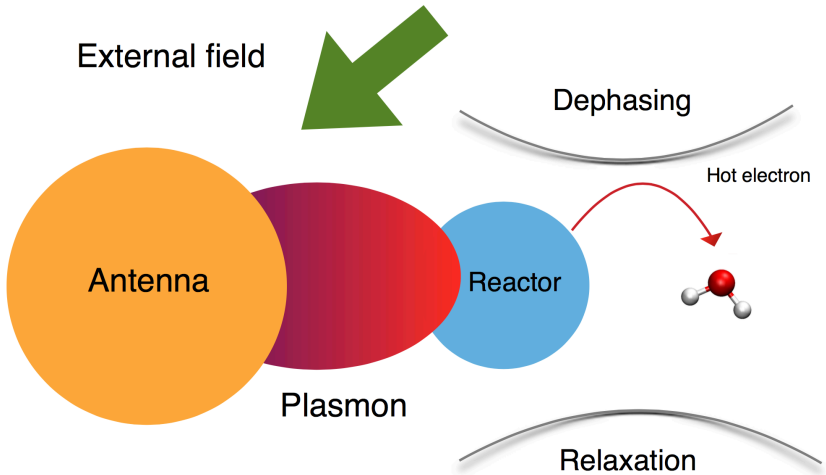
1. Hot-carrier generation and dynamics
2. Hydrogen formation in antenna-reactor complexes
3. Theory: Stochastic time-dependent Schrödinger equation (SSE) (quantum coherence)





Theory of open quantum systems: SSE





ARTICLE

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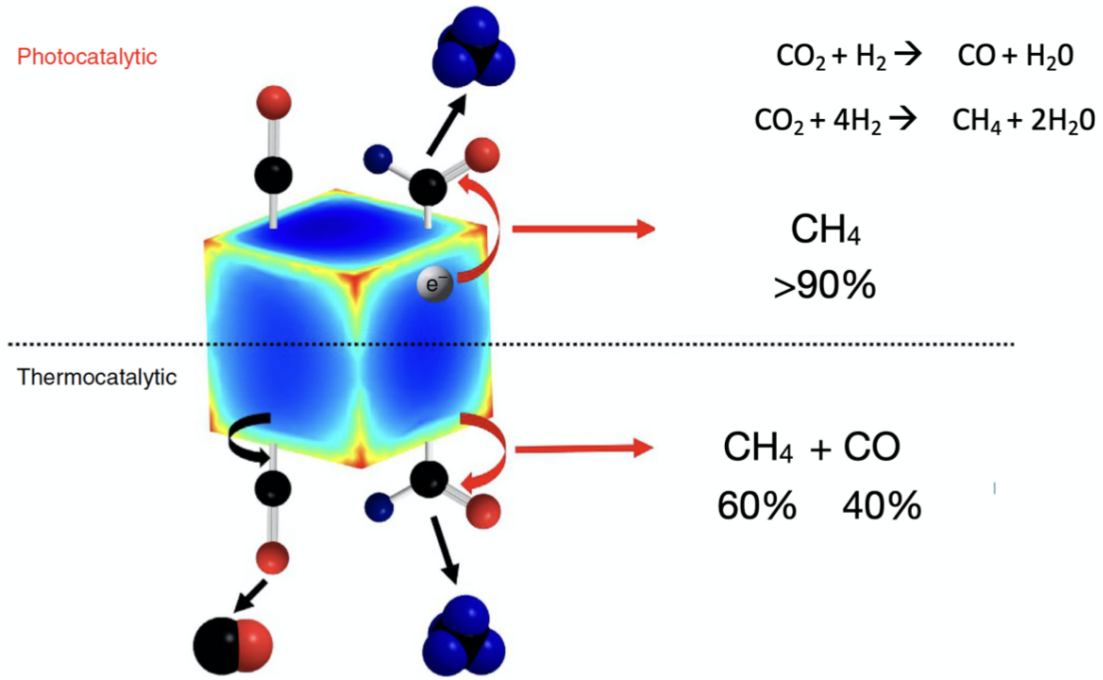
Product selectivity in plasmonic photocatalysis for carbon dioxide hydrogenation

Xiao Zhang[1], Xueqian Li[1], Du Zhang[1], Neil Qiang Su[1], Weitao Yang[1], Henry O. Everitt[2,3] & Jie Liu[1]



Selectivity enhancement due to hot carriers?

X. Zhang, X. Li, D. Zhang, N. Q. Su, W. Yang, H. O. Everitt and J. Liu, *Nat. Commun.*, **8**, 14542 (2017)

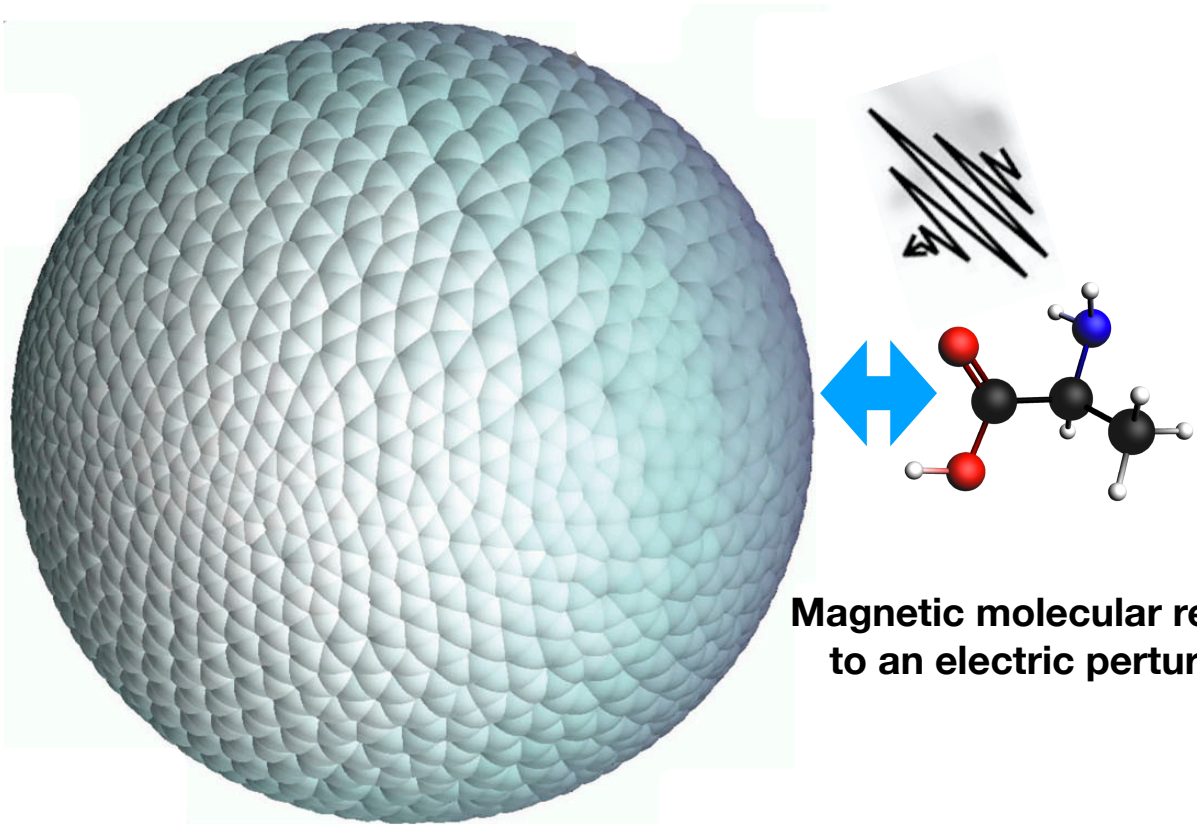
Theoretical modelling of plasmon-assisted electronic circular dichroism (ECD)

Collaboration with Università di Padova
one PhD student (Leonardo Biancorosso)

Theoretical modelling of plasmon-assisted electronic circular dichroism (ECD)

Collaboration with Università di Padova
one PhD student (Leonardo Biancorosso)

1. How the plasmonic nanoparticle affects the ECD spectrum?
2. Application to amino acids
3. excited-state ECD of gas-phase molecules
4. Theory: coherent time-dependent Schrödinger equation and SSE



Magnetic molecular response to an electric perturbation

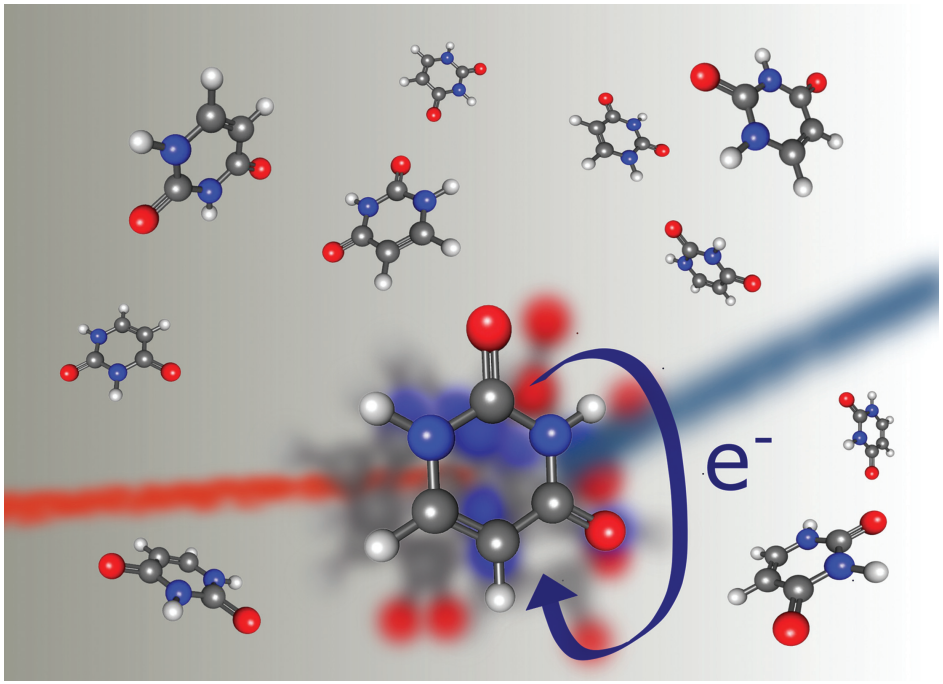
Strong-field electron dynamics in molecules under the influence of intense laser pulses: high-harmonic generation (HHG) spectroscopy

Collaboration with Sorbonne Universitè (Paris), University of Nova Gorica, Politecnico di Milano and Universidad Autonoma de Madrid
one PhD student (Chiara Morassut)

Strong-field electron dynamics in molecules under the influence of intense laser pulses: high-harmonic generation (HHG) spectroscopy

Collaboration with Sorbonne Universitè (Paris), University of Nova Gorica, Politecnico di Milano and Universidad Autonoma de Madrid
one PhD student (Chiara Morassut)

1. Study of orbital symmetry with tailored fields
2. Circular dichroism in HHG spectra of chiral molecules
3. Plasmon-assisted HHG
4. Theory: time-dependent Schrödinger equation with complex energies
5. Close interaction with experimentalists



Showcasing research from the Theoretical Chemistry Group of University of Trieste, Italy (Emanuele Coccia), and Laboratoire de Chimie Théorique of Sorbonne Université, France (Eleonora Luppi)

Probing the molecular frame of uracil and thymine with high-harmonic generation spectroscopy

This work shows recent advances in simulating high-harmonic generation (HHG) spectra on biomolecules such as uracil and thymine. Wave-function methods and dynamics are coupled for generating and propagating the all-electron wavepacket interacting with an intense infrared pulse. Ionisation step in both molecules probably involves orbitals other than HOMO. HHG spectra with a pulse polarisation perpendicular to the molecular plane differ in the cutoff region from those by a three-dimensional average.

As featured in:

See Eleonora Luppi and Emanuele Coccia, *Phys. Chem. Chem. Phys.*, 2021, **23**, 3729.

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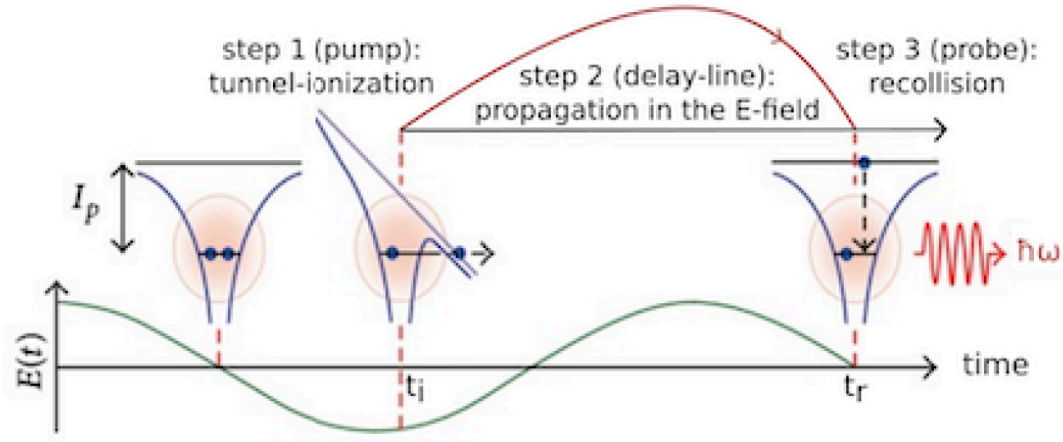
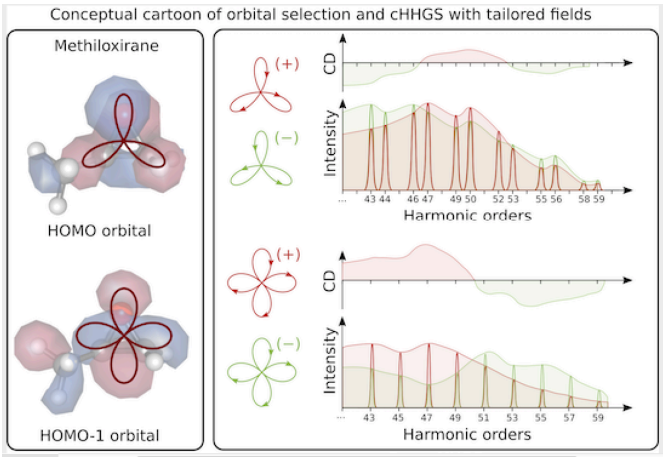
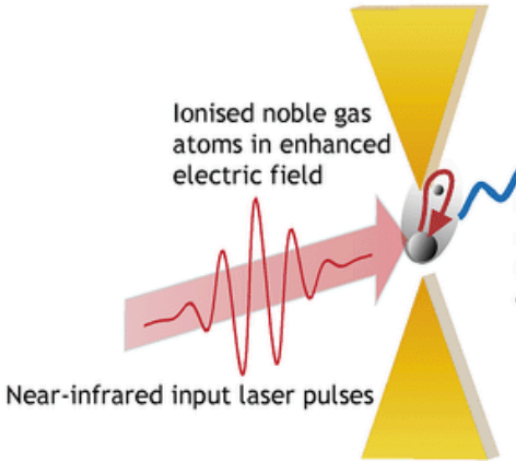

step 1 (pump):
tunnel-ionization
step 2 (delay-line):
propagation in the E-field
step 3 (probe):
recollision
I_p
$\hbar\omega$
$E(t)$
time
t_i
t_r


Conceptual cartoon of orbital selection and cHHGS with tailored fields
Methiloxirane
HOMO orbital
HOMO-1 orbital
(+)
(−)
CD
Intensity
43 44 46 47 49 50 52 53 55 56 58 59
Harmonic orders
43 45 47 49 51 53 55 57 59
Harmonic orders


Ionised noble gas
atoms in enhanced
electric field
Near-infrared input laser pulses