

# Master thesis projects

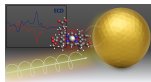
Emanuele Coccia

Dipartimento di Scienze Chimiche e Farmaceutiche

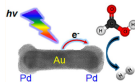


## PhotoInduced Quantum Dynamics Unit

### Molecular plasmonics

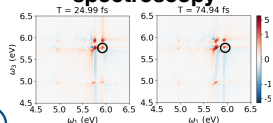


Enhanced CD



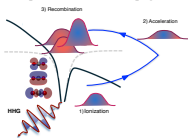
Photocatalysis

### Two-dimensional electronic spectroscopy

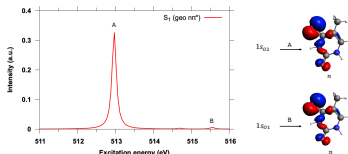


Time-domain  
quantum mechanics  
(electrons)

### High-harmonic generation spectroscopy



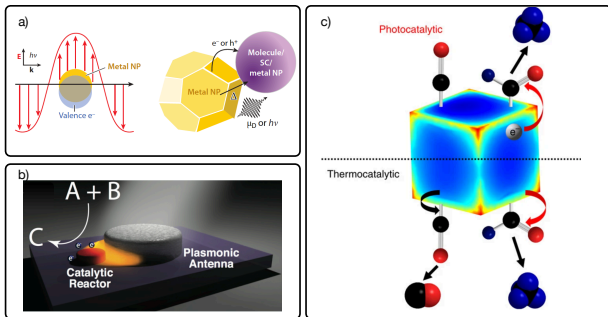
### X-ray spectroscopies



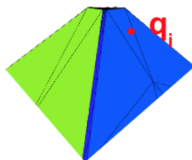
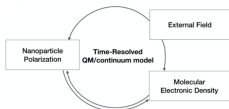
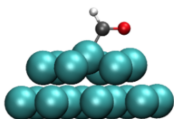
# Theoretical modelling of plasmon-assisted photocatalysis

Collaboration with Università di Padova, Bologna, King's College in London (UK), Lorraine University in Metz (France)

- 1 Hot-carrier generation and dynamics
- 2 Novel reaction pathways
- 3 Enhanced production rate
- 4 Enhanced product selectivity



# Time-domain QM/continuum approach



## Time-dependent Schrödinger equation

$$i\frac{\partial|\Psi(t)\rangle}{\partial t} = \hat{H}(t)|\Psi(t)\rangle$$

$$\hat{H}(t) = \hat{H}_0 - \vec{\mu} \cdot \vec{E}_{ext}(t) + \mathbf{q}(t)\mathbf{V}$$

$$|\Psi(t)\rangle = \sum_{\lambda} C_{\lambda}(t)|\lambda\rangle$$

$$|\lambda\rangle = \sum_i \sum_{\alpha} d_{i,\lambda}^{\alpha} |\Phi_i^{\alpha}\rangle$$

## EOM for surface charges

$$\mathbf{q}(\omega) = \frac{1}{2\pi} f(\omega)\mathbf{F}(\omega)$$

$$f(\omega) = \frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 1}$$

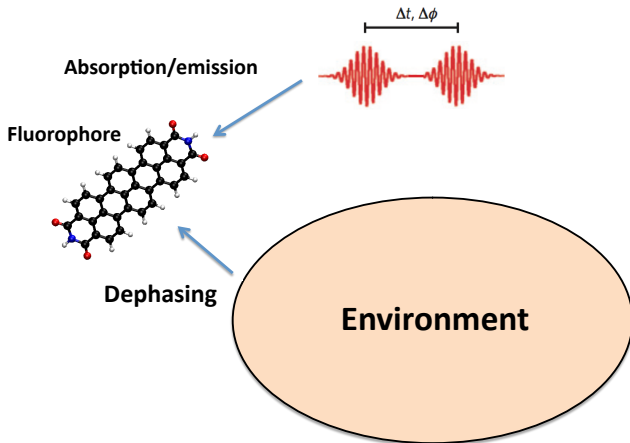
$$\mathbf{F}(\omega) = -[\mathbf{AD}^* \mathbf{q}(\omega) + \mathbf{S}^{-1}(2\pi\mathbf{I} + \mathbf{DA})\mathbf{V}(\omega)]$$

$$\ddot{\mathbf{q}}(t) = -\gamma\dot{\mathbf{q}}(t) - \mathbf{Q}_{\omega}\mathbf{q}(t) + \mathbf{Q}_f\mathbf{q}(t)$$

Real-time simulations with polarizable continuum model (RT-PCM-NP)

# Theory of open quantum systems

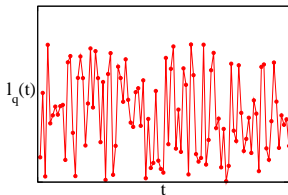
Collaboration with Sorbonne University in Paris and Lorraine University in Metz (France)



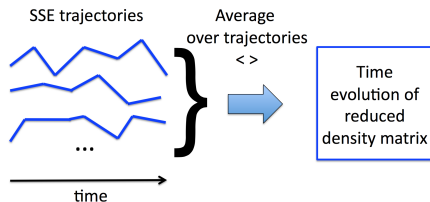
# Stochastic Schrödinger equation (SSE)

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle + \sum_q I_q(t)\hat{S}_q|\Psi(t)\rangle - \frac{i}{2}\sum_q \hat{S}_q^\dagger\hat{S}_q|\Psi(t)\rangle$$

$$|\Psi(t)\rangle = \sum_\lambda C_\lambda(t)|\lambda\rangle$$



## • SSE in Markovian limit

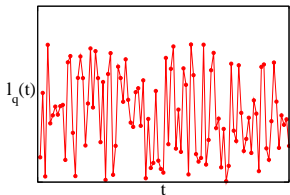


## • Why SSE?

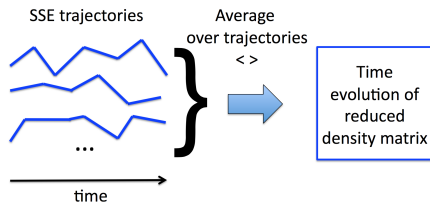
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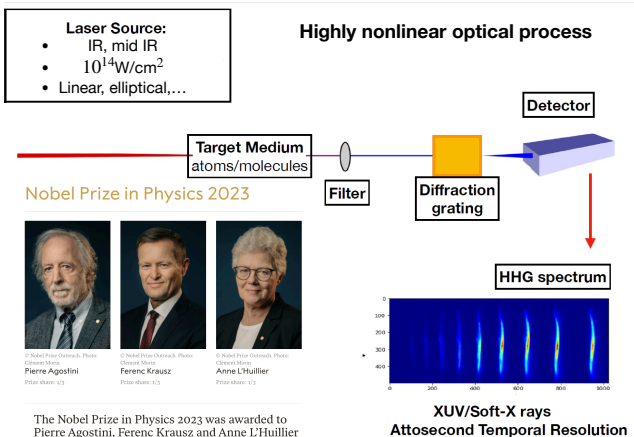
## • SSE in Markovian limit



- Why SSE?
- Studying decoherence (2DES)
- Effective dynamics in complex systems

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

Collaboration with Sorbonne Université (Paris), University of Nova Gorica, CNR in Milan, MPI in Berlin (Germany) and King's College in London (UK)

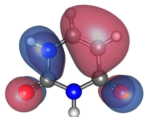


# Theoretical framework

## QUANTUM CHEMISTRY

$$\hat{H} = \hat{T}_e + \hat{T}_N + \hat{V}_{eN} + \hat{V}_{ee} + \hat{V}_{NN}$$

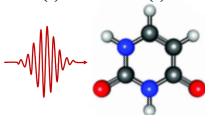
$$\Psi(\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_N)$$



## TIME PROPAGATION

$$i \frac{\partial \Psi(t)}{\partial t} = \hat{H}(t) \Psi(t)$$

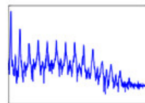
$$\hat{H}(t) = \hat{H} + \hat{V}(t) + \hat{I}$$



## HHG SPECTRUM

$$\vec{\mu}(t) = \langle \Psi(t) | \vec{\mu} | \Psi(t) \rangle$$

$$\text{FT}(\vec{\mu}(t) \cdot \vec{n}_\alpha)$$

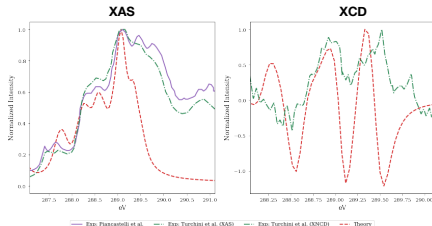
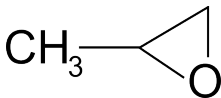
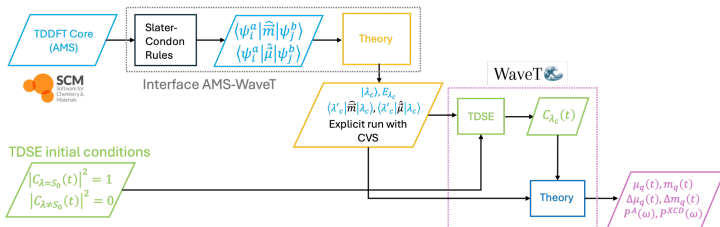


Light

# X-ray spectroscopies using time-domain quantum chemistry

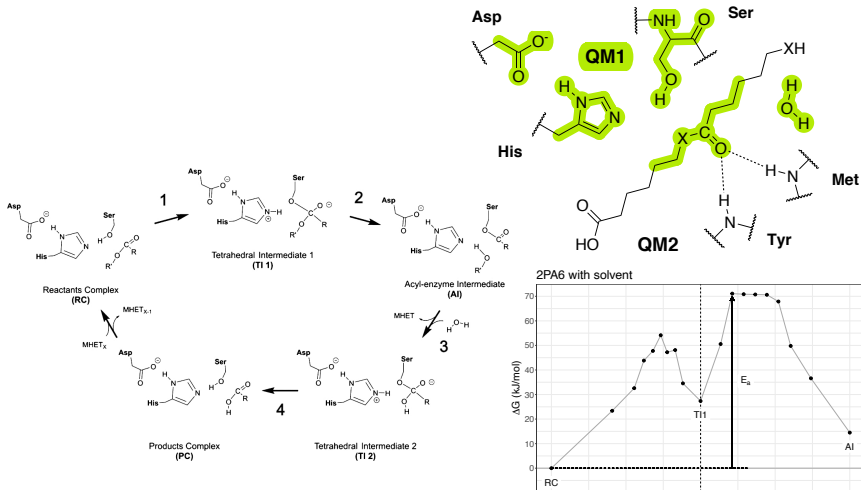
Collaboration with Elettra and EPFL in Lausanne (Switzerland)

- 1 Spin-orbit coupling for thiouracil (X-ray absorption)
- 2 X-ray circular dichroism



# Multiscale simulations for enzymatic reactions

Collaboration with Rita De Zorzi





# Quantum Monte Carlo methods

Collaboration with University of Twente (The Netherlands)

