

Coupled Electron-Nuclear Dynamics for Electron Capture Processes

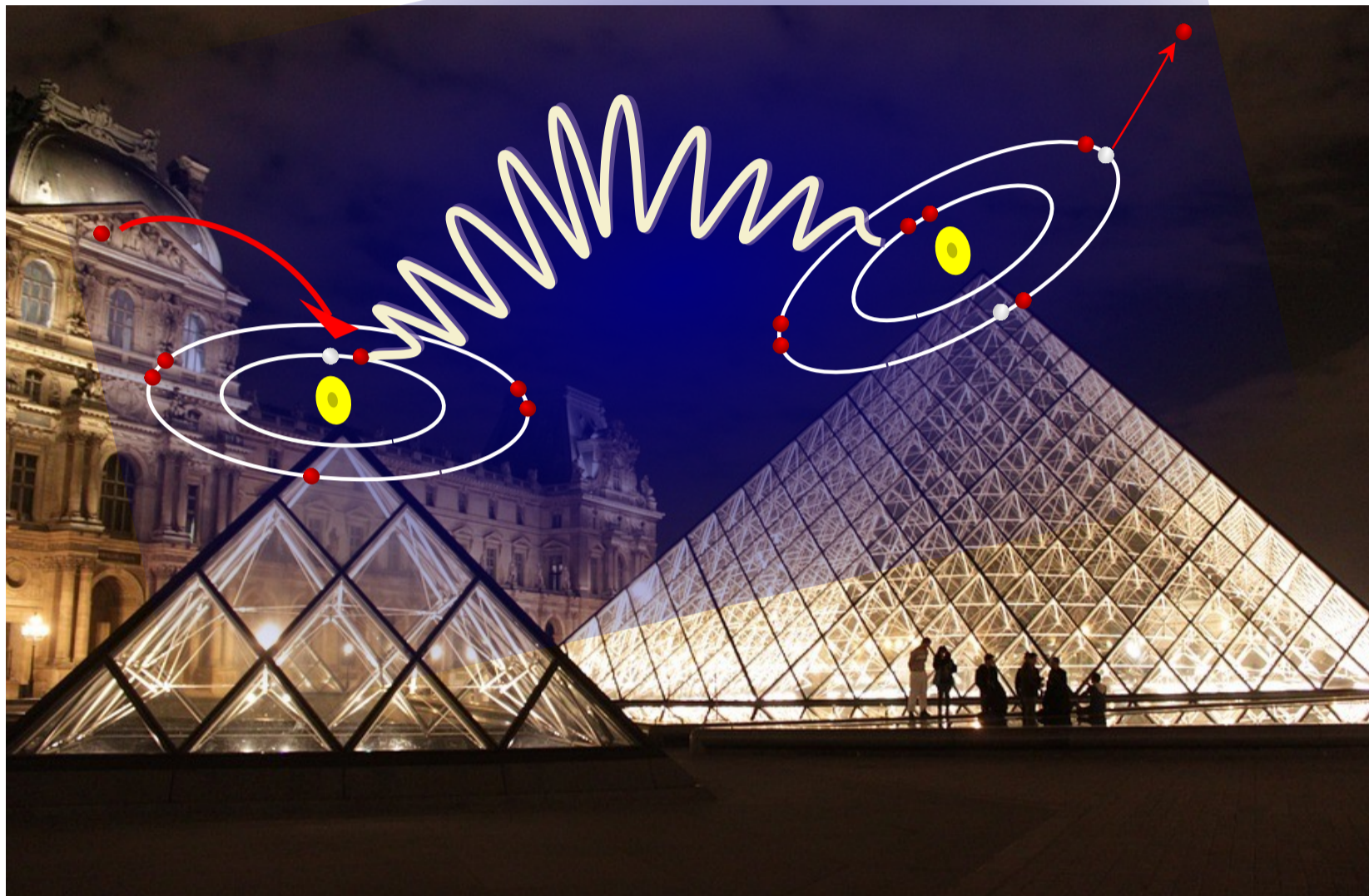
Paris, 15-16 February 2023

Organizing Committee:

Annika Bande
Elke Fasshauer
Axel Molle
Daniel Peláez
Federico Pont
Nicolas Sisourat

Funding:

QD4ICEC



Inter-particle Coulombic electron capture (ICEC) is an environment-enabled process in which an electron can be efficiently attached to an ion, atom, molecule, or quantum dot. The excess energy is simultaneously transferred to a neighboring system which undergoes ionization. ICEC has been predicted by theoretical approaches ranging from analytical models to ab-initio electronic structure and dynamical calculations. Their common assumption is that nuclei remain fixed during ICEC. However, given the time scale of ICEC, nuclear dynamics should play an important role in changing the efficiency and/or influencing the final state of the system. The aim of our workshop is to discuss original quantum-dynamical methods to provide a complete description of ICEC.

Register at qd4icec.sciencesconf.org



Venue:

On-site: Campus Pierre et Marie Curie,
4 Place Jussieu, Paris, France

Virtual participation: the link will be provided shortly before the event

Contact:

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Program

Wednesday, Feb. 15

13:30 Welcome and Coffee

14:00 Lorenz S. Cederbaum

Interparticle Coulombic Electron Capture

14:45 Axel Molle/Nicolas Sisourat

R-matrix and Virtual Photon Approximation

16:00 Annika Bande/Federico Pont

Dynamical simulations of ICEC using MCTDH

16:45 Elke Fasshauer/Daniel Peláez

tba,

Analytical representation of operators for quantum dynamical simulations

Thursday, Feb. 16

9:00 Loïc Joubert-Doriol

tba

9:45 Přemysl Koloreňč

Fano-ADC with B-splines

11:00 Petr Slavicek

tba

11:45 Morgane Vacher

Non-adiabatic dynamics and on-the-fly methods

14:00 Françoise Remacle

Controlling quantum dynamics through electronic entanglement in molecules pumped by ultrashort optical pulses

14:45 Jimena Gorfinkiel

Nuclear motion in R-matrix studies of electron scattering

16:00 Fernando Martín

Effect of nuclear motion on the electron dynamics generated by attosecond pulses in molecules



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We hope to welcome you in Paris or online!