Production of reactive oxygen species for ultrafast plasmon therapy: role of the optical near field

by

Syrine Gueffrache

directed by
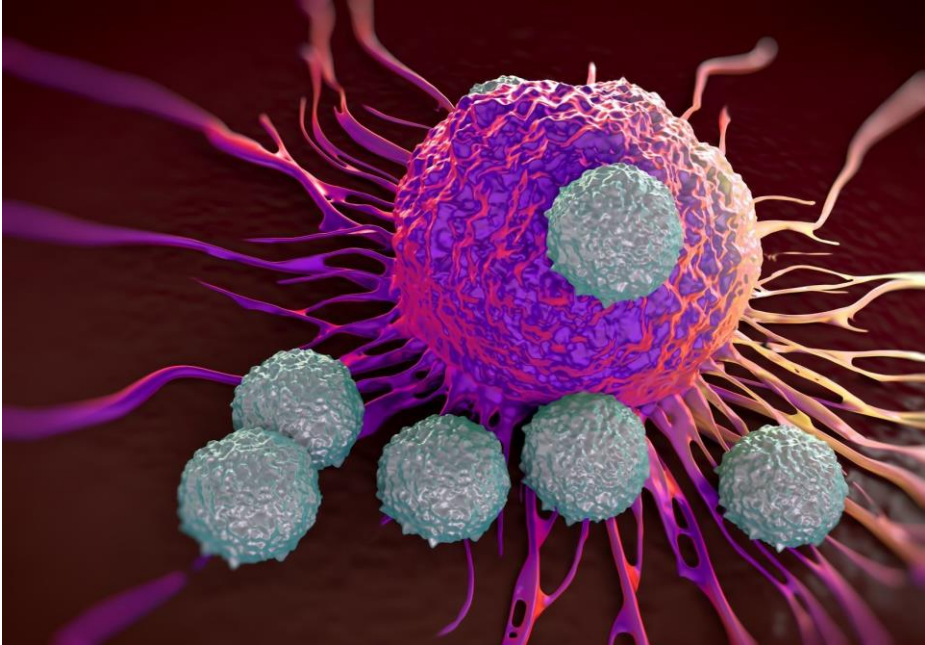
Bruno Palpant, LuMIn laboratory

Labex NanoSaclay 13/10/2020

Cancer: An international concern...

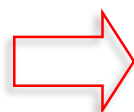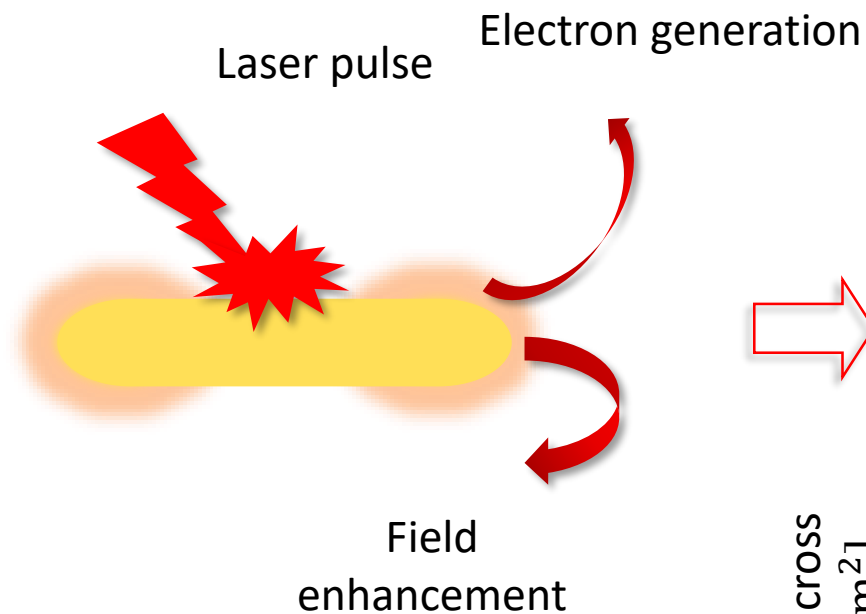
Organisation mondiale de la Santé

✓ More than 8 millions deaths in the world in 2015

✓ 15 millions people will be affected in 2020

✓ Chemical therapy, radiotherapy, photodynamic therapy

✓ Several disadvantages: hair loss, cardiac failure, etc.

✓ Why? Lack of localized therapy

✓ Gold nanoparticles

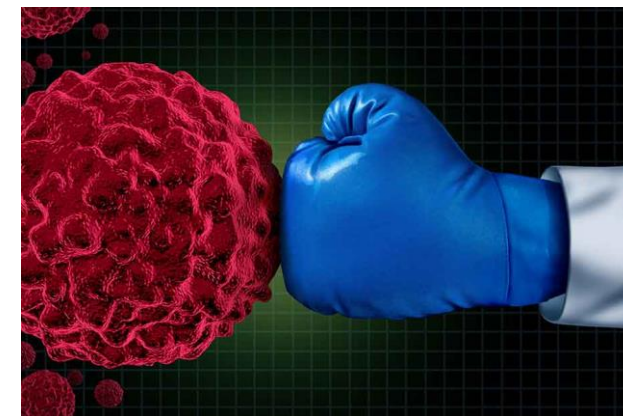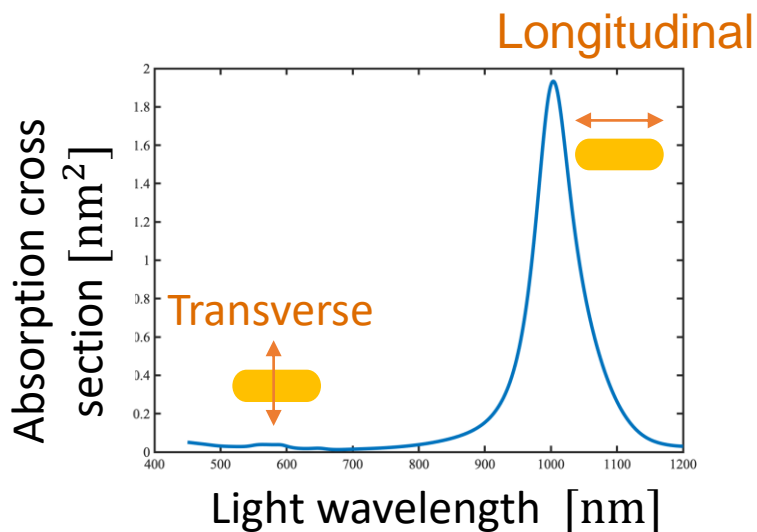# Gold nanoparticles and their optical effect
What we already know

Laser pulse

Electron generation

Field enhancement

Localised surface plasmon resonance

Superoxide $O_2^{\cdot -}$
Hydrogen peroxide H_2O_2
Hydroxyl radical $\cdot OH$
Singlet oxygen $^1O_2$

Reactive Oxygen Species for cancer treatment

Longitudinal

Transverse

Absorption cross section [nm^2]

Light wavelength [nm]

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Gold nanoparticles and their optical effect
What we already know

Laser pulse

Electron generation

Field enhancement

Localised surface plasmon resonance

Optical properties of gold evolve during the pulse duration

Longitudinal

Transverse

Absorption cross section [nm^2]

Light wavelength [nm]
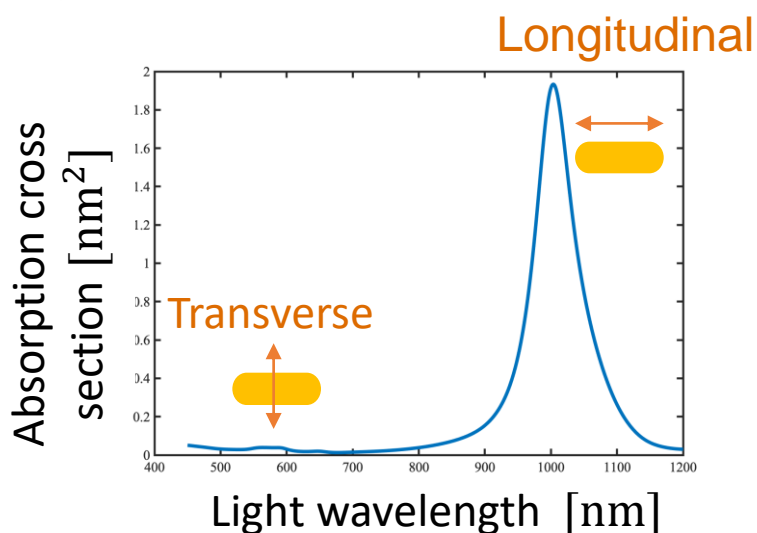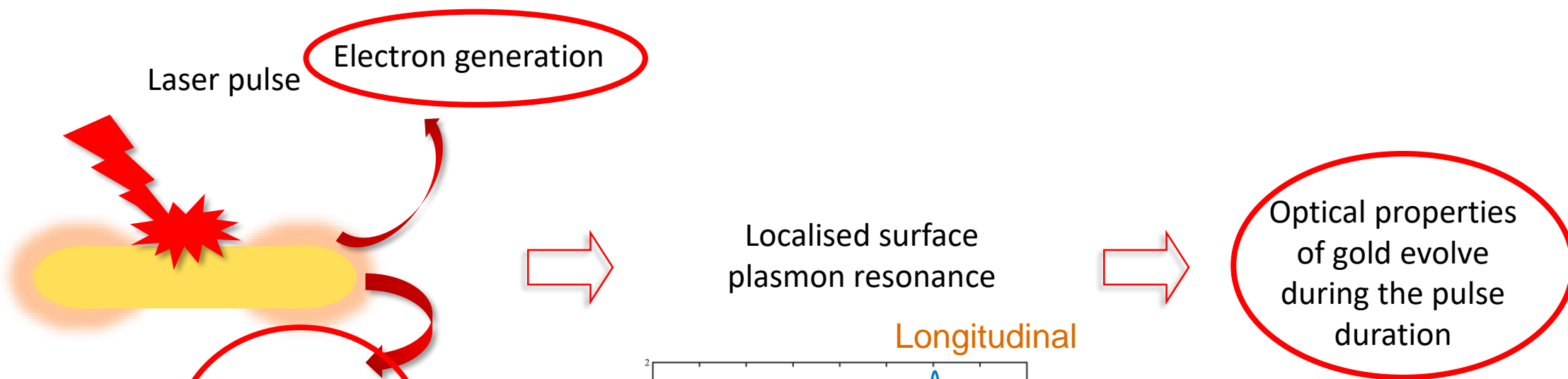
Efficient Multiphoton Plasmonic Production of Reactive Oxygen Species: who are we?

Sylvie Marguet, chemist, CEA

Synthesis of gold nanoparticles

Christophe Leboeuf, biologist, INSERM

In vivo studies of tumor regression by laser irradiation

EMPPROS
Coord. Bruno Palpant

Ludovic Douillard, physicist, CEA

Fundamental study of the light-triggered electron emission from the plasmonic objects by PEEM

Guilhem Bousquet, oncologist, Hôp. Avicennes

Robert Pansu, chemist, ENS Paris-Saclay

Study of ROS production via fluorescence probe microscopy

Syrine Gueffrache, Ph.D student, CentraleSupélec
Numerical simulations: dynamics of the field topography in vacuum, electron generation in biological medium
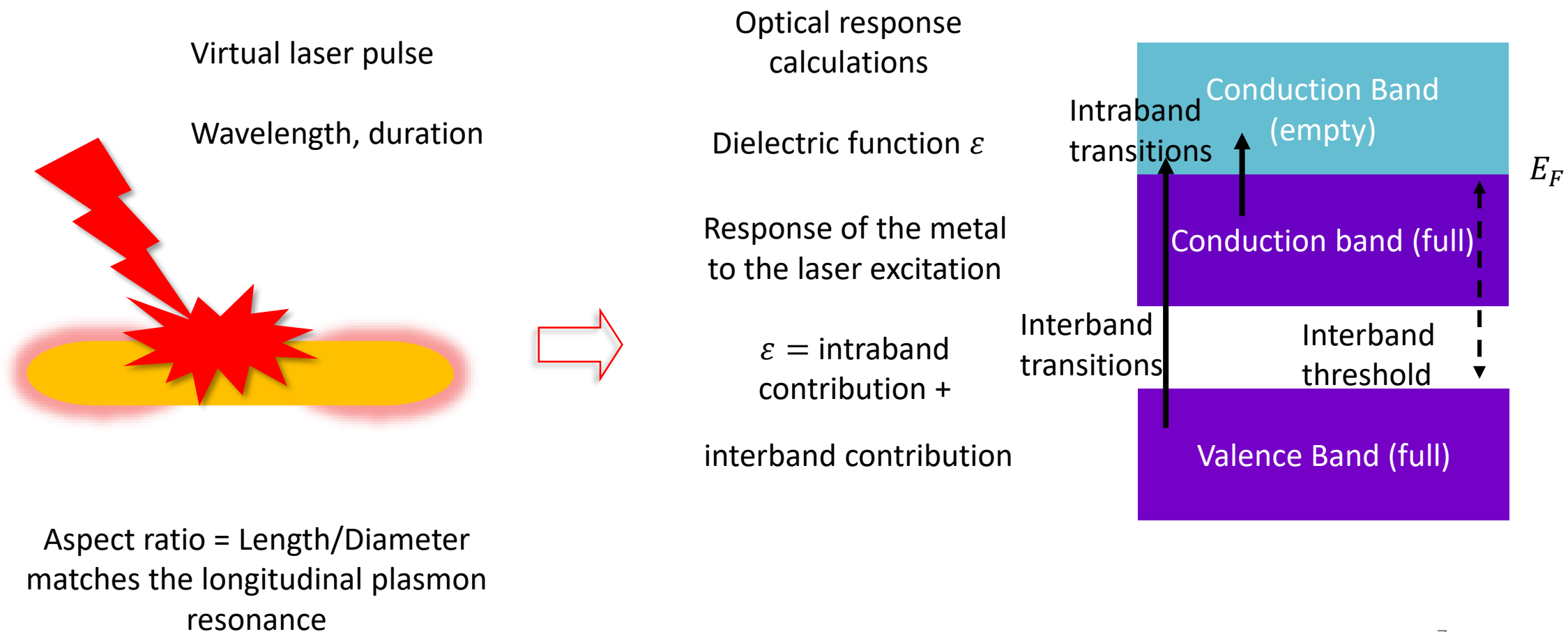Experiments: *in vivo* tumor irradiation, dynamics of solvated electrons
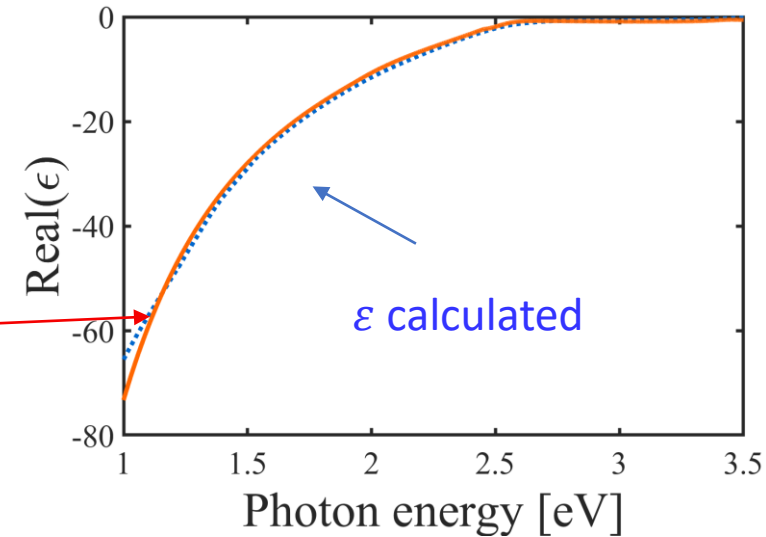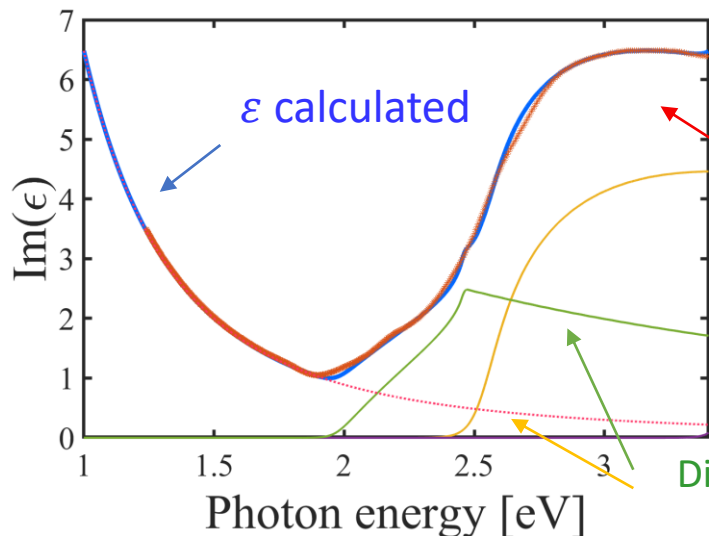
What am I doing in my theoretical part…

✓ Optical response of the gold nanoparticles and its dynamical evolution in the non-equilibrium state (hot electrons)

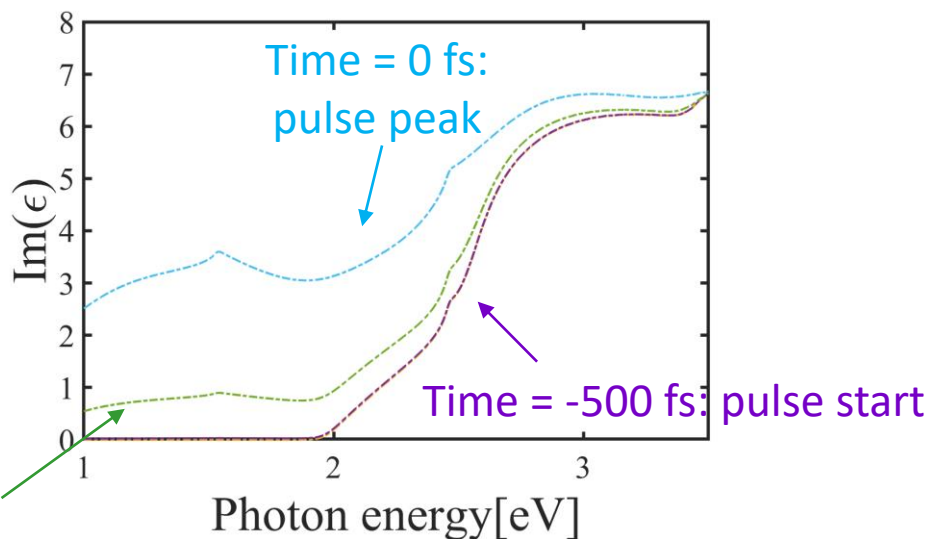✓ Dynamics of the topography of the optical near-field throughout the duration of the laser pulse.

# Numerical calculations of the optical dielectric function

Virtual laser pulse

Wavelength, duration

Optical response calculations

Dielectric function ε

Response of the metal to the laser excitation

ε = intraband contribution +

interband contribution

Intraband transitions

Conduction Band (empty)

E_F

Conduction band (full)

Interband transitions

Interband threshold

Valence Band (full)

Aspect ratio = Length/Diameter matches the longitudinal plasmon resonance

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Dielectric function's calculation

ε calculated

Experimental ε

Different contributions to ε

ε calculated

Dynamical evolution of the interband contribution to the dielectric function
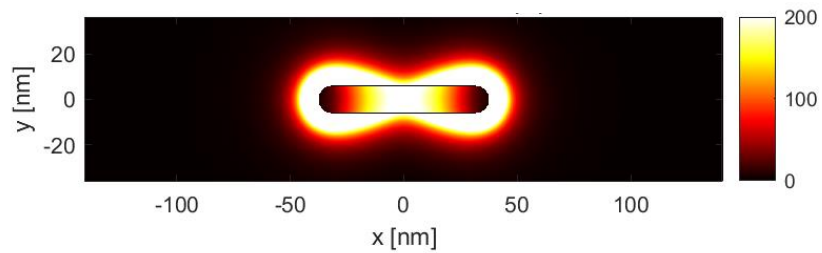

Time = 0 fs: pulse peak
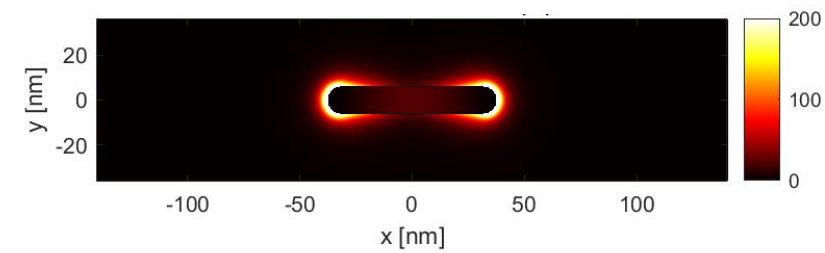
Time = -500 fs: pulse start

Time = -100 fs

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For the experimental detection of solvated electrons:
Application to a 12 nm x 75 nm nanorod in water irradiated by a 1030-nm, 234-fs laser pulse
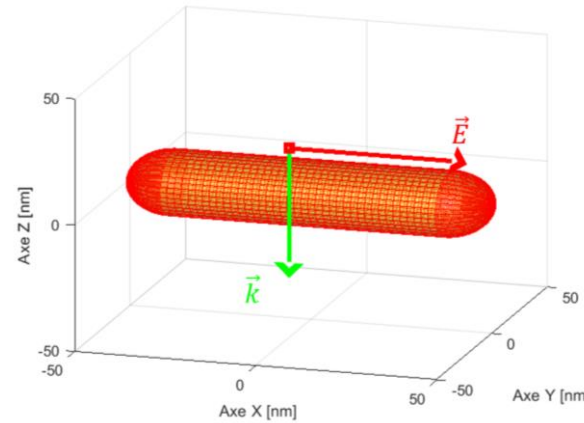
Intensity $\left|\vec{E}\right|^{2}$ at the beginning of the pulse
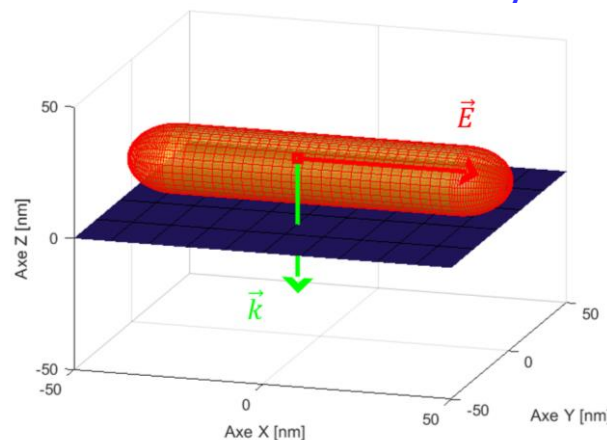

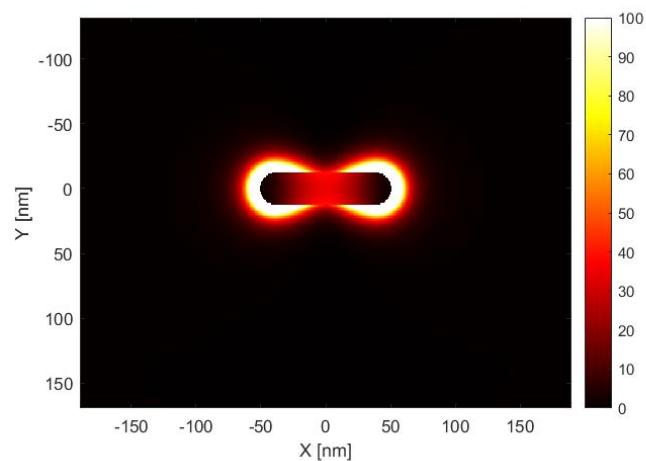Intensity $\left|\vec{E}\right|^{2}$ at the end of the pulse

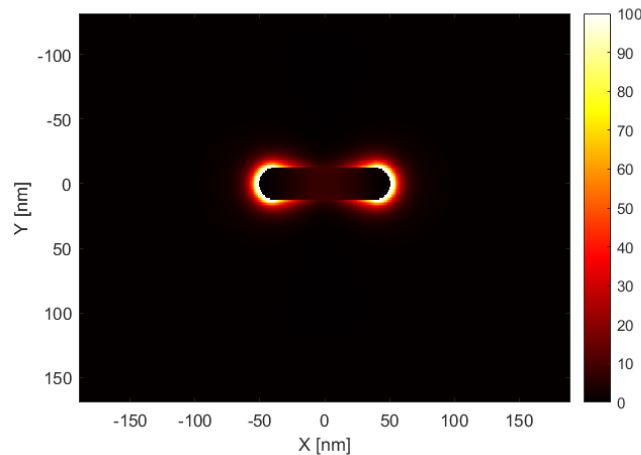For the analysis of the PEEM experiment in SPEC/CEA: Gold nanorod on ITO substrate
Application to a 25 nm x 101 nm nanorod in vacuum irradiated by 791 nm pulse laser with a pulse duration of 154 fs
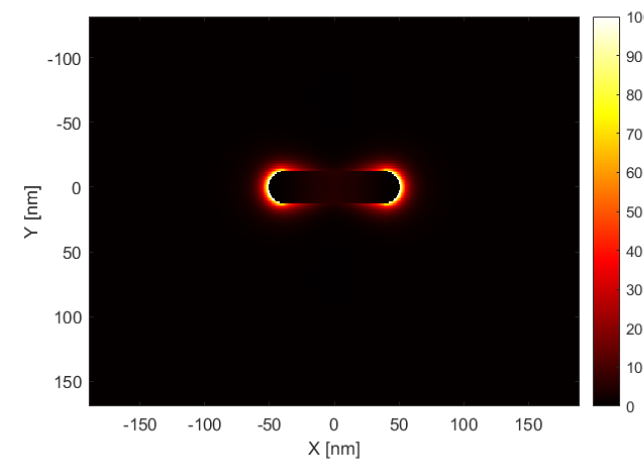

Intensity $\left|\vec{E}\right|^{2}$ at the beginning of the pulse

Intensity $\left|\vec{E}\right|^{2}$ at the middle of the pulse

Intensity $\left|\vec{E}\right|^{2}$ at the end of the pulse

✓ Dynamics of the athermal response in the non-equilibrium regime that enables us to obtain the ultrafast dynamics of the near-field topography

✓ Dynamics of the field will enable us to access the kinetics and topography of the electrons ejected

In vivo studies: protocol

Tumor
Xenograph

Gold
nanoparticles
injection

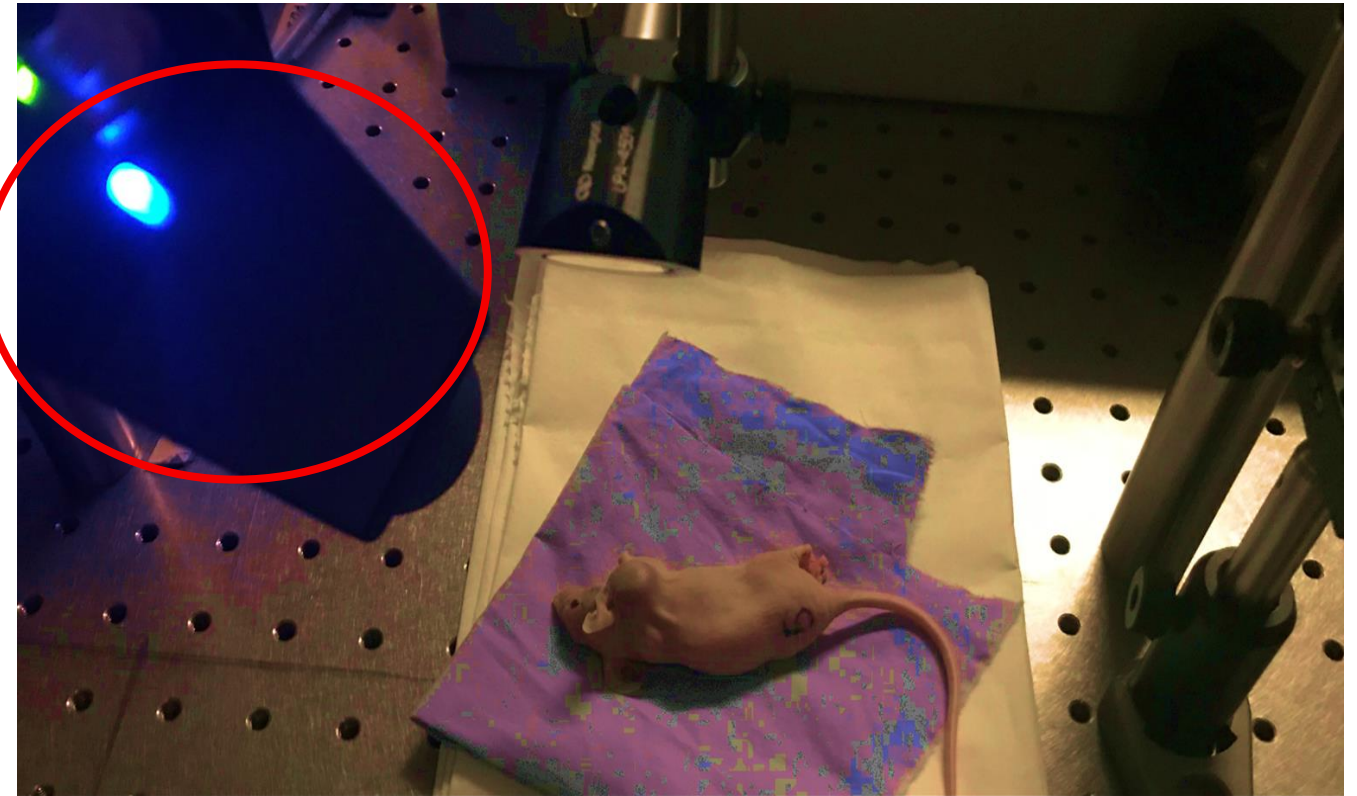Laser
irradiation
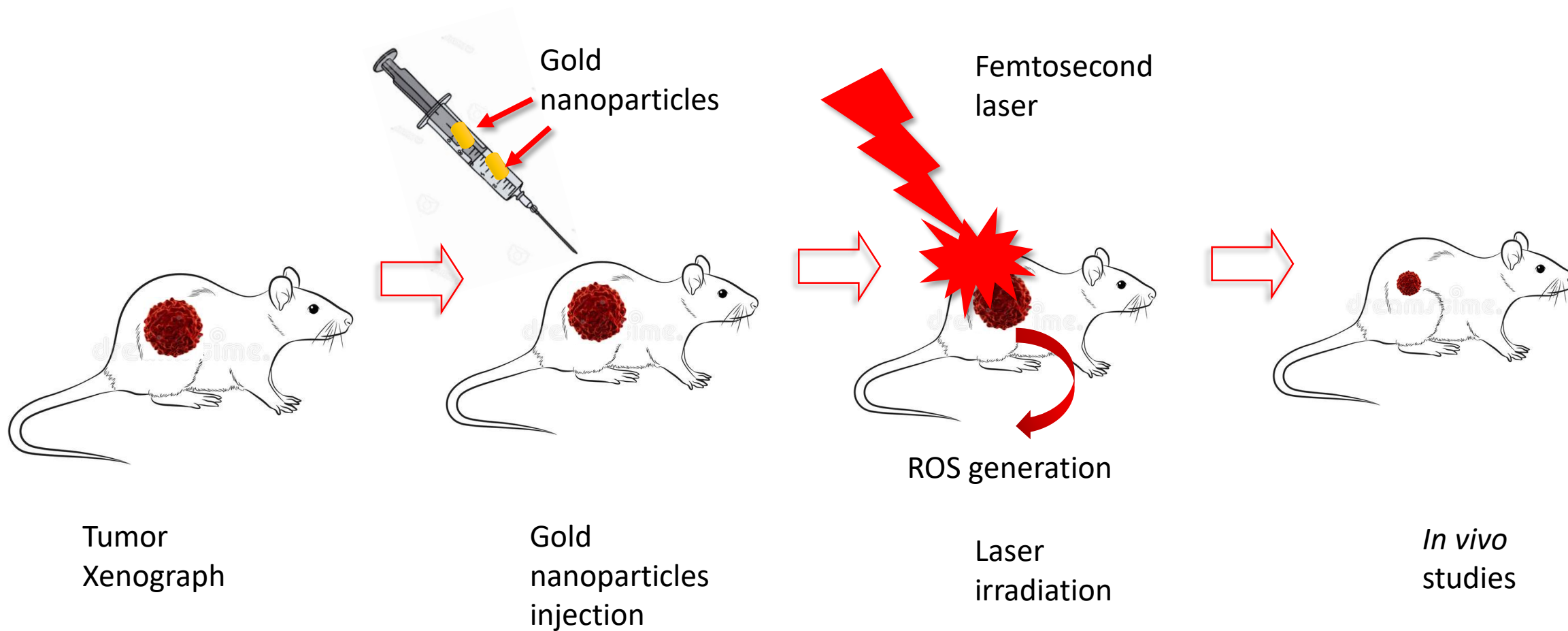
In vivo
studies

In vivo studies: protocol

Irradiation setup
Femtosecond laser
Pulse duration = 234 fs, $\lambda = 1030$ nm

Mouse with triple negative human breast cancer
+ gold nanorods

Thank you for you attention

Any questions?