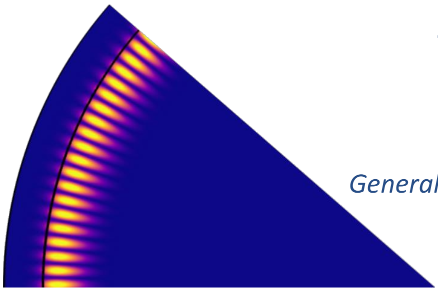
COMSOL Day 2020
University of Duisburg-Essen

Nanoplasmonic and Nanophotonic simulations



Mandana Jalali, Daniel Erni

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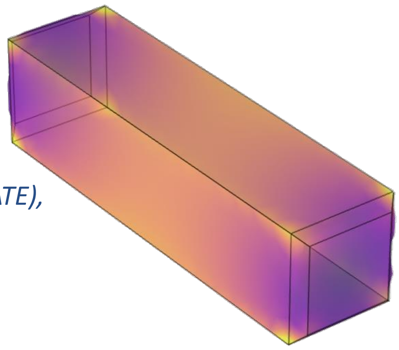
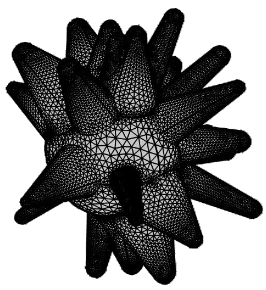
https://www.ate.uni-duisburg-essen.de



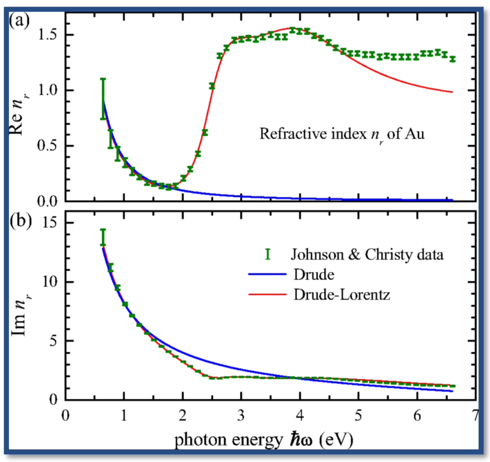
Nano Optical devices:

Why using FEM method?



- ❖ Unstructured mesh
- ❖ High accuracy
- ❖ Dispersive behavior of plasmonic material

➡ At the end we pay for the expensive required computational resources



E. Muljarov, et al. Phys. Rev. B. 93, (2015).

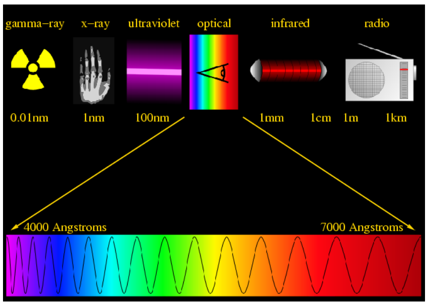
Nano Optical devices:

Why using FEM method?

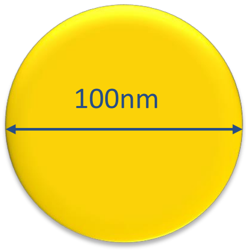
- Unstructured mesh
- High accuracy
- Dispersive behavior of plasmonic material

We use *COMSOL* Wave Optics Module, which provide proper measure to account for the electrical size ($\frac{L_C}{\lambda}$) of the modelling object.

Nano Optical Simulations:

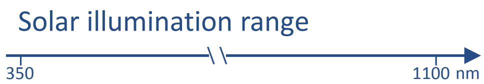


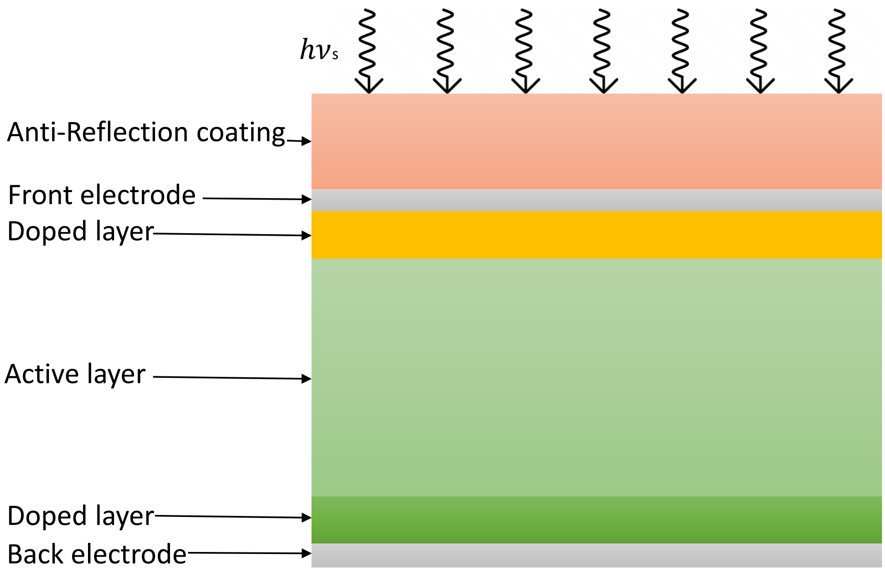
$400 - 700nm$



Solar Cell- Thin film c-Si:

An ultra-broadband optical device





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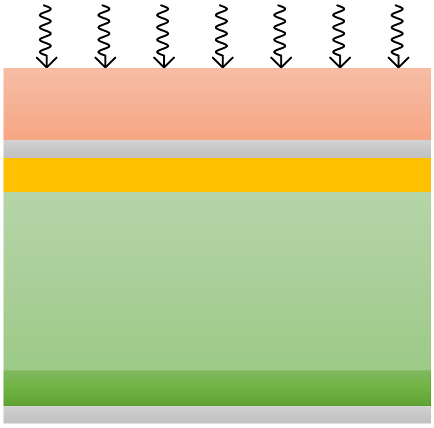
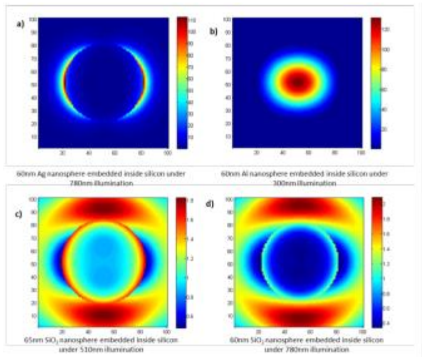


Optical design:

- ❖ What fraction of light reaches the active layer?
- ❖ What is the spectral range of the corresponding light?
- ❖ What is the absorption probability?
- ❖ What techniques to use to increase the absorption probability?



M. Jalali, et al. Proc. of ICNS5. (2014).

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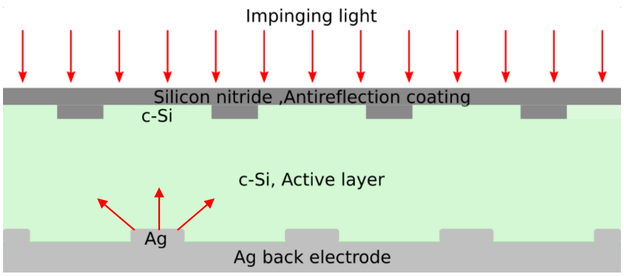
Solar Cell:

An ultra-broadband optical device

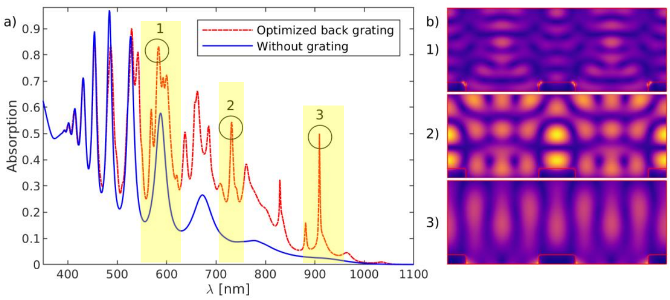
Plasmonic back-grating



- ❖ Design and optimize a plasmonic back-grating
- ❖ Excite some well-defined mode within the active layer

However:

- Reflection is still rather high
- The optical path is quite short



M. Jalali, et al, Crystals, **9**(5), 264. (2019).

Solar Cell:

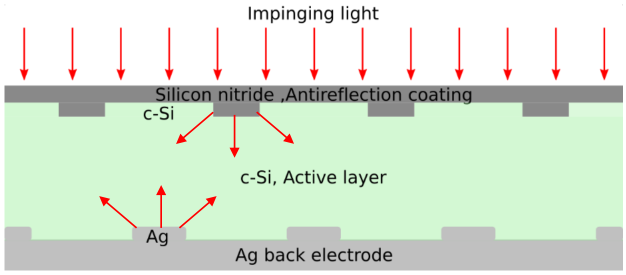
An ultra-broadband optical device

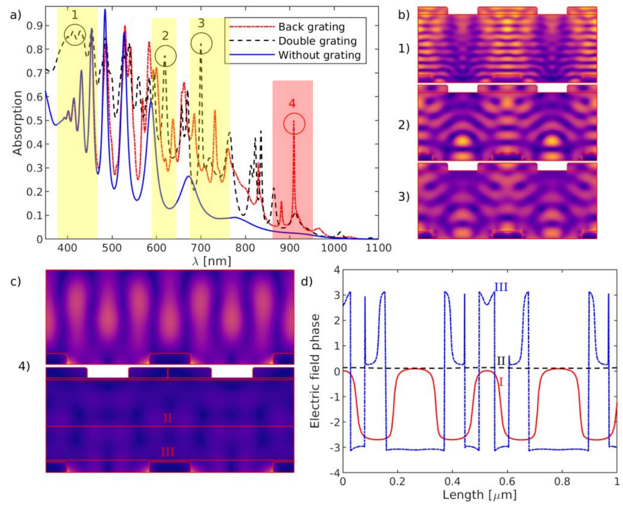
Adding an optimized front-grating

- ❖ Add a front-grating from the same material as the active layer
- ❖ Injects the light diffusely to the active layer
- ❖ When designed in a smart manner, constructive coupling to the back-grating

However:

- ▪ We still just get some well-defined modes each corresponding to a peak in the absorption spectra





M. Jalali, et al, IJOP, **11**(2), 79-86. (2017).

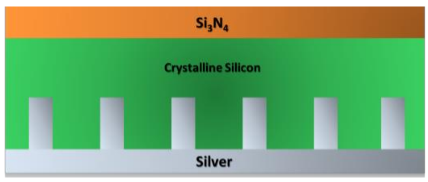
Solar Cell:

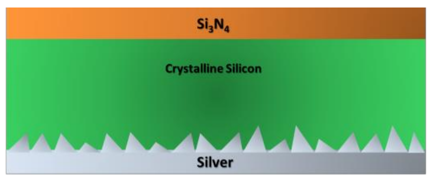
An ultra-broadband optical device

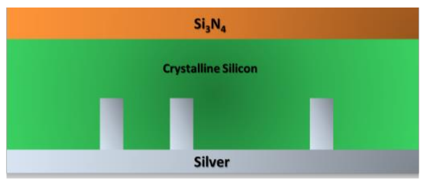
Semi-periodicity: an apt solution

Why semi-periodicity?

- ❖ Periodic structures create distinct, strong peaks in the absorption spectrum
- ❖ Random structures create a lot of weak peaks
- ❖ Semi-periodicity: a trade off between peak number and peak strength







M. Jalali, et al, J. Nanophotonics, **10**(3), 036018. (2016).

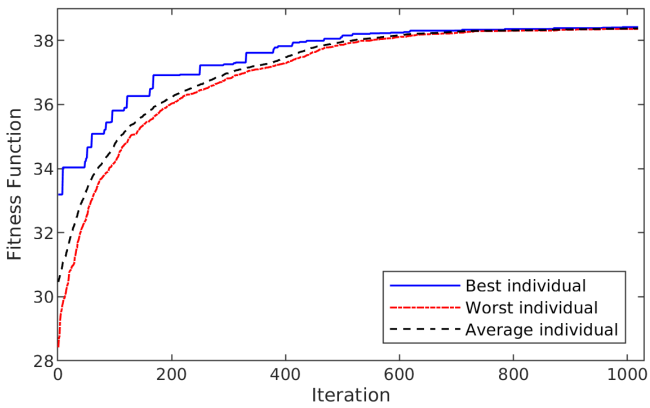
Solar Cell:

An ultra-broadband optical device

Semi-periodicity: an apt solution

How to define:

- Based on numerical structural optimization
- The optimized grating teeth parameters are kept constant
- A 32 binary sequence is randomly defined and subjected to optimization



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Solar Cell:

An ultra-broadband optical device

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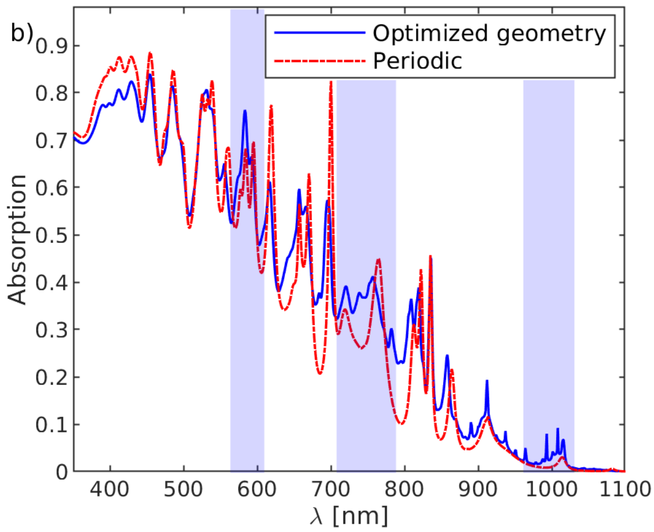
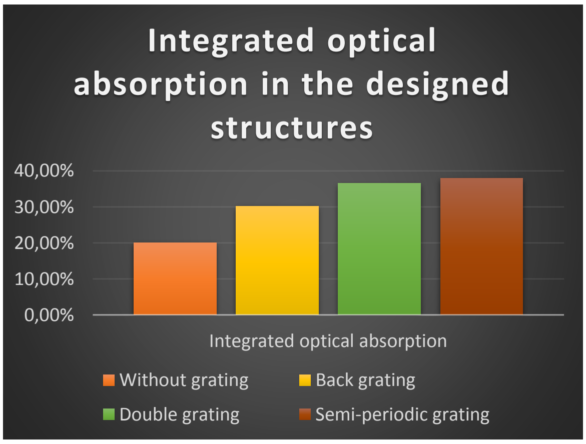


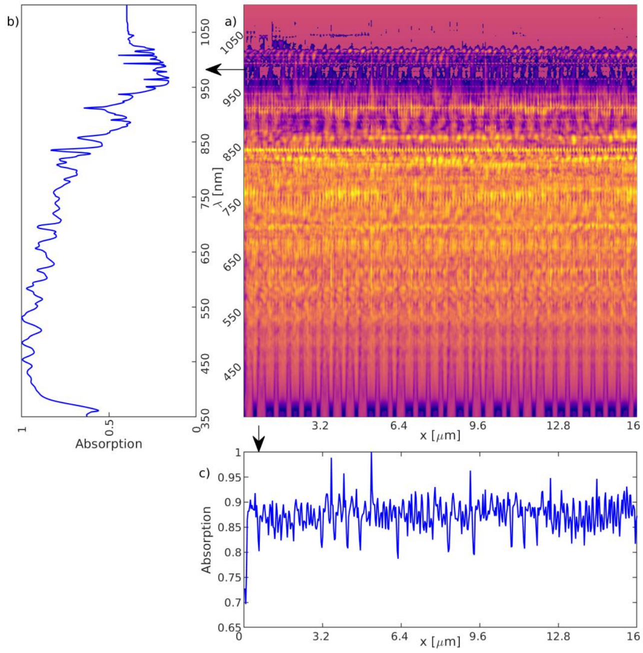
M. Jalali, et al, J. Nanophotonics, **10**(3), 036018. (2016).

Solar Cell:

An ultra-broadband optical device

Semi-periodicity: Does it work?



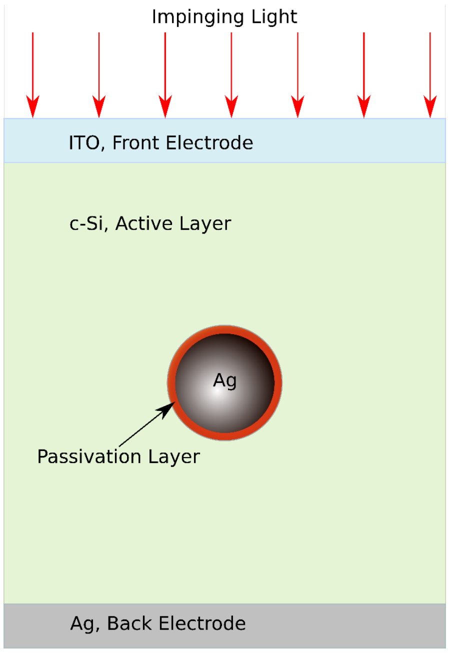


M. Jalali, et al, Crystals, **9**(5), 264. (2019).

Solar Cell:

Electronic properties

- Studying electronic as well as optical properties of the solar cell
- Mixing the wave optic module with the semiconductor module
- However:
- Simplified 2D models are tractable
- Solving 3.27×10^5 degrees of freedom which takes about 9h on a Core i7 computer with 64GB of RAM



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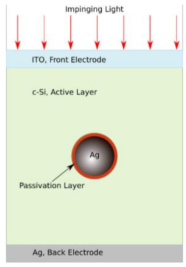
Solar Cell:

Electronic properties



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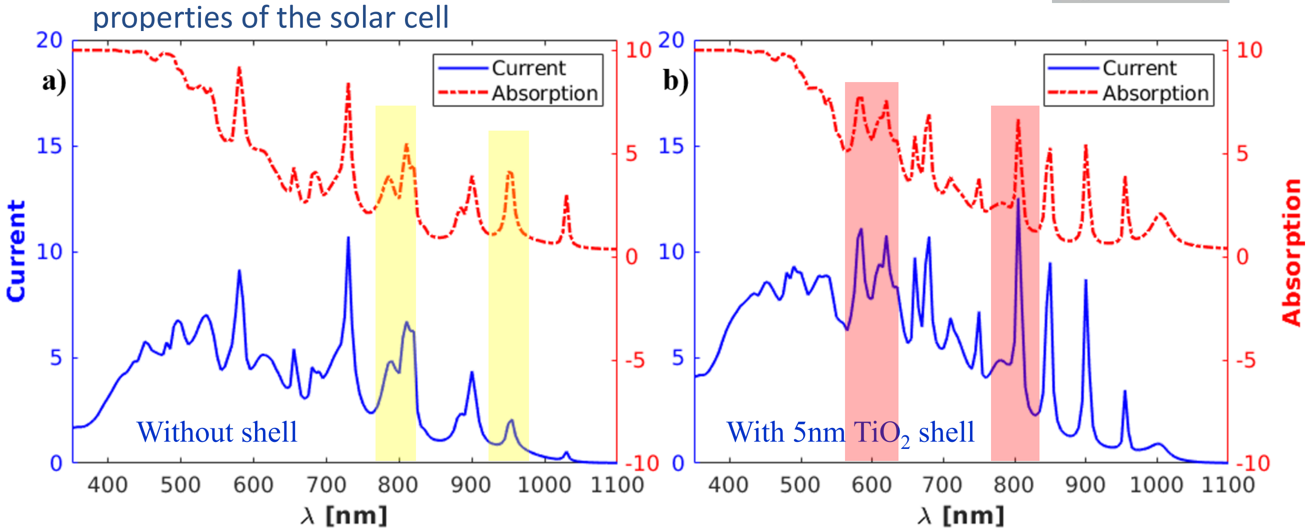

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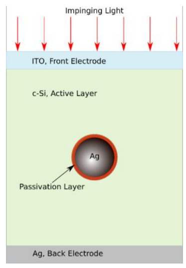
Solar Cell:

Electronic properties



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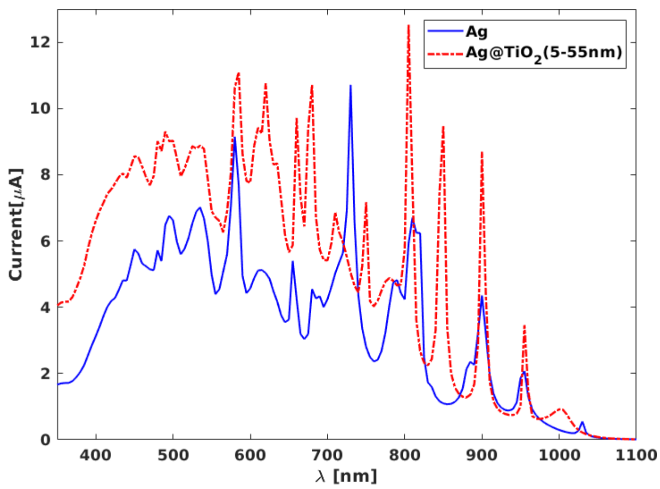

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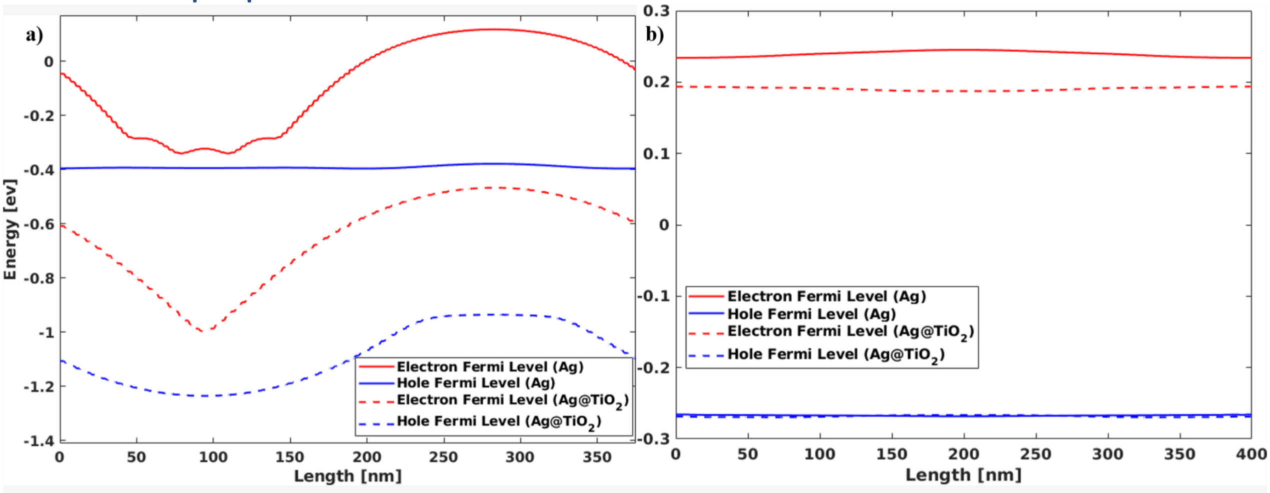
Solar Cell:

Electronic properties



Quasi-Fermi energy levels at an operating wavelength of 395nm around Ag NP in presence and absence of 5nm TiO_2 shell as a function of the arc length of the particle's circumference, and at the edge of the active layer.

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Solar Cell:

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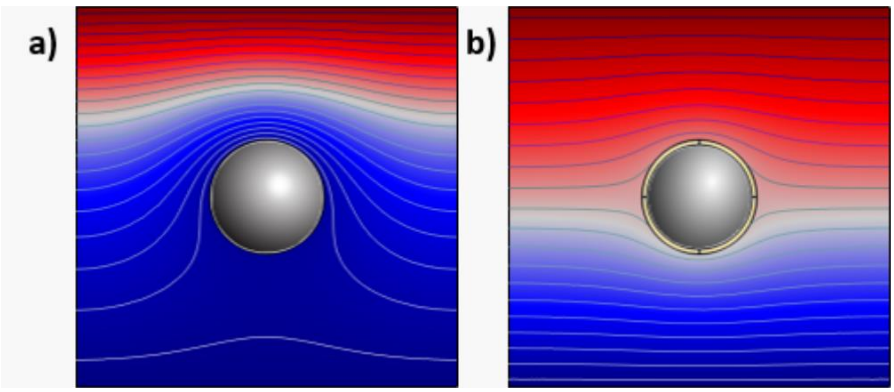
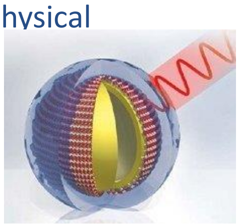
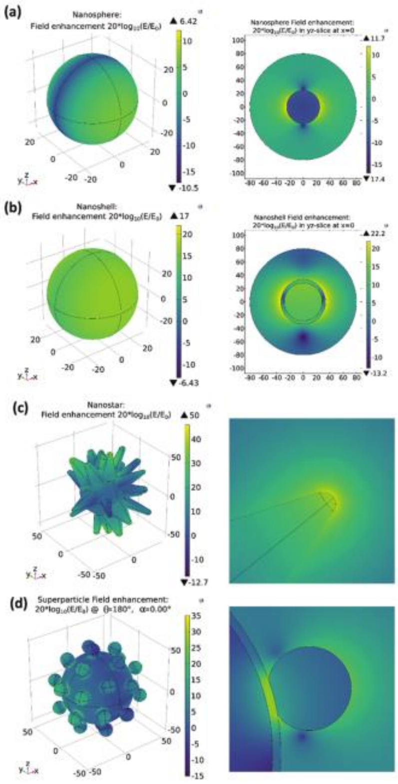


Surface Enhanced Raman Scattering (SERS), single-particle level:

- Different classes of plasmonic nanoparticles functionalized with non-resonant Raman reporter molecule 4-MBA are simulated for their SERS signal brightness at the single particle level.
- This work has been done in collaboration with the Physical chemistry group

Physical Chemistry
Prof. Dr. Sebastian Schlücker





V. Tran, C. Thiel, J. T. Svejda, M. Jalali, B. Walkenfort, D. Erni, & S. Schlücker, Nanoscale, **10**(46), 21721-21731 (2018).

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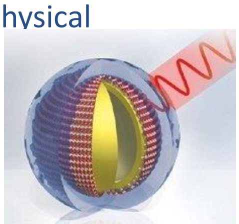

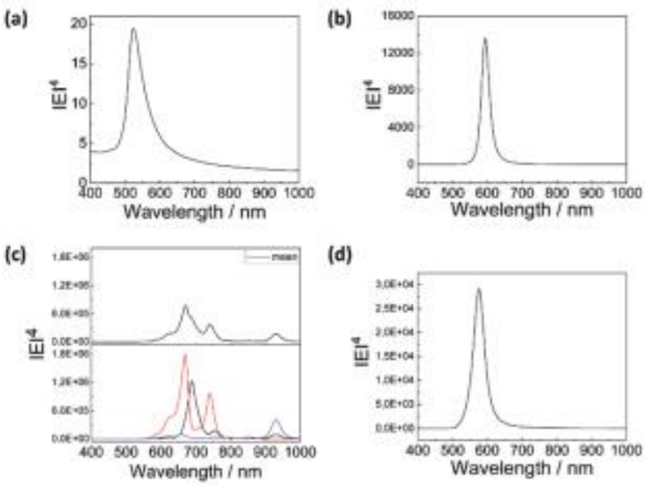

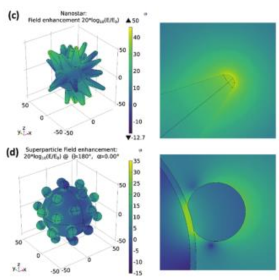

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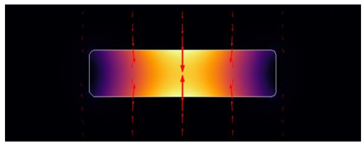
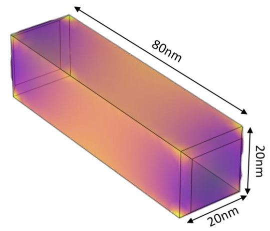
Nano-Bio-Plasmonics:

Nano-Bio-Plasmonics is implementing nanoplasmonics in *Bio* applications such as sensitive sensors, hyperthermia, bio-imaging and …

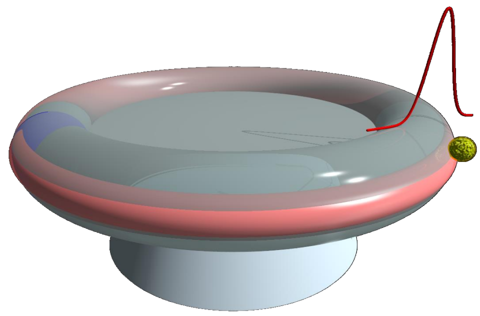
- The challenge lies in proper modelling the bio environment at nanoscale
- Often requires *Multiphysics* simulation, with the appropriate connection between optics and the bio system

Gold nanoparticle-mediated-hyperthermia





Ultra-sensitive biosensors based on micro resonators



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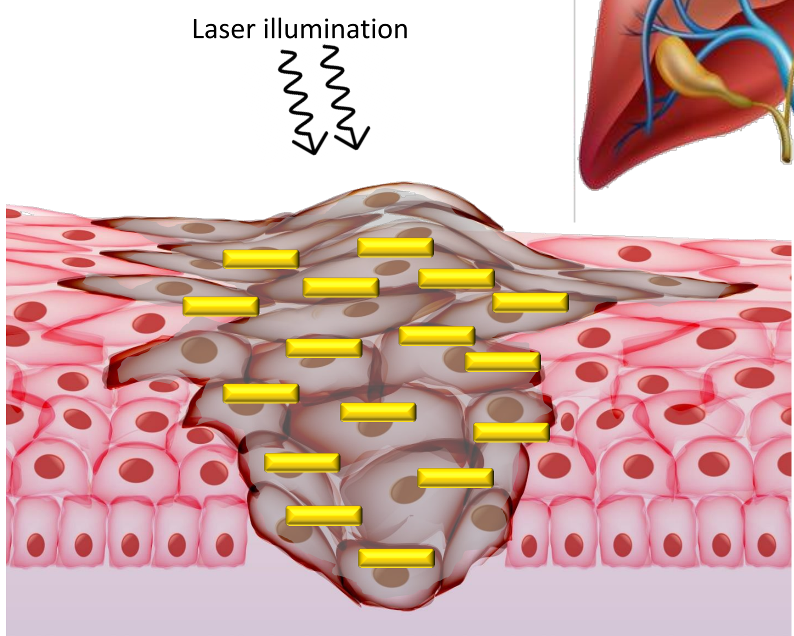
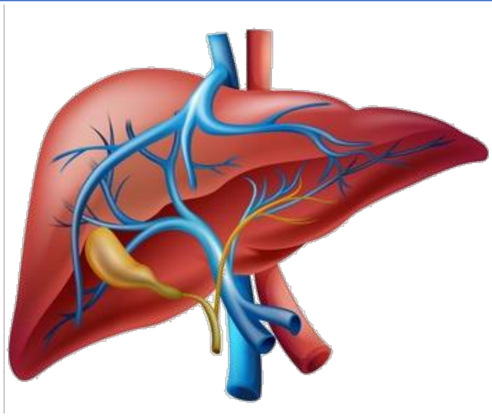
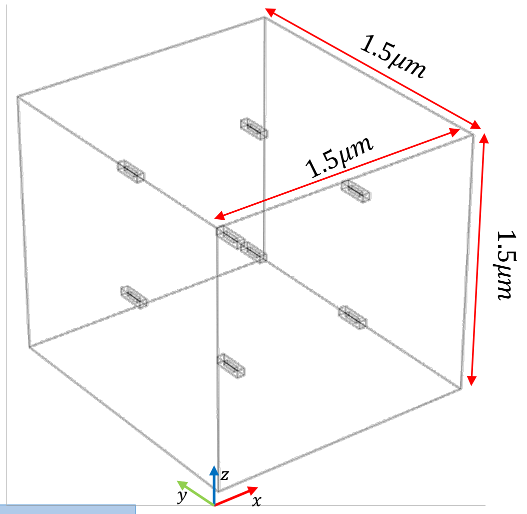




Gold nanoparticle-mediated-hyperthermia

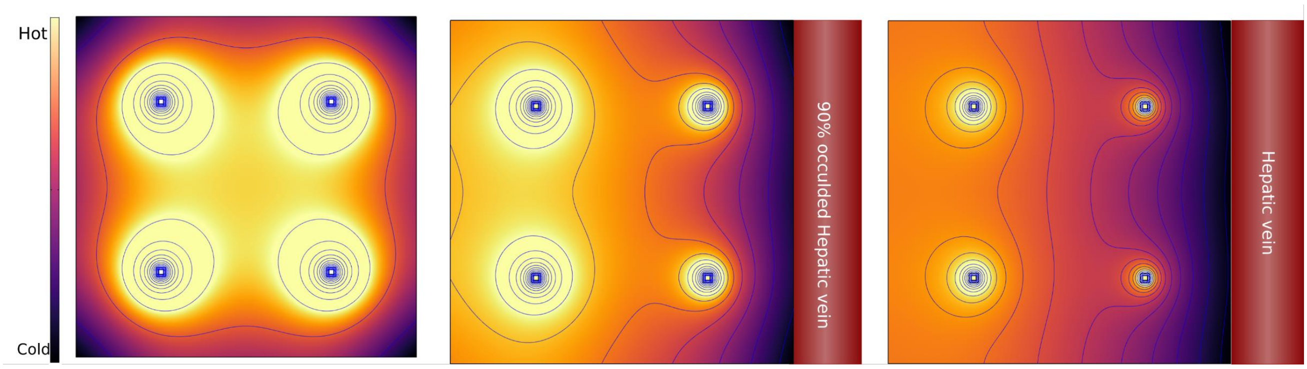
We have set-up a model based on mixing wave optics module with bio heat transfer module to study the effect of veins on hyperthermia



Plane wave is illuminated to the pNPs at the optimized resonance frequency, considering a mean medium for liver tissue → Heat transfer in the liver tissue and temperature enhancement → Account for cooling through blood flow

M. Jalali, et al, Int. Conf. Appl. Opt. & Photonics, **11207**, 112070M (2019).

Gold nanoparticle-mediated-hyperthermia



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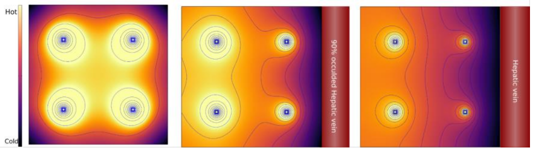
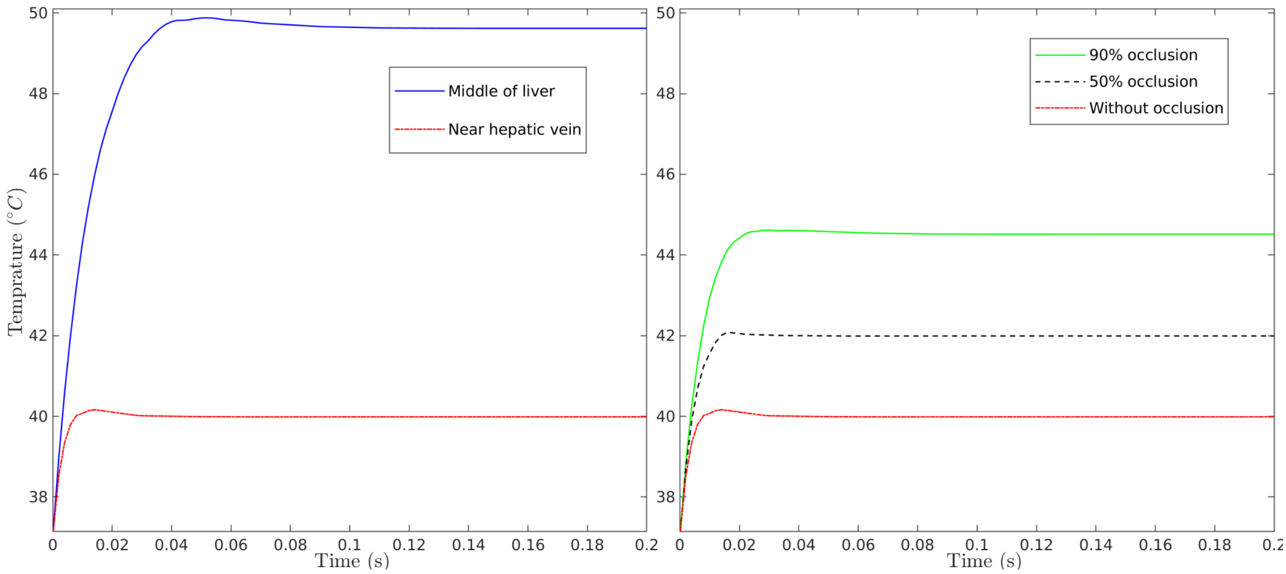


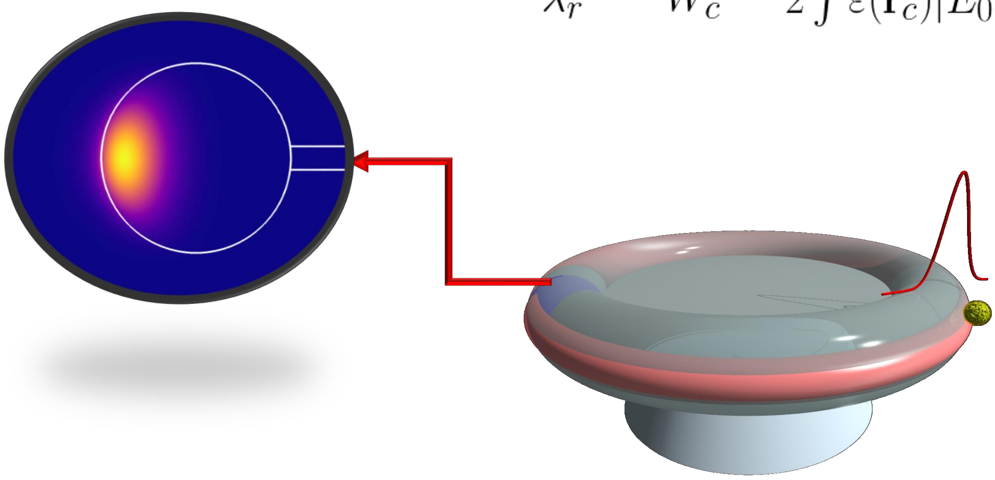


M. Jalali, et al, Int. Conf. Appl. Opt. & Photonics, **11207**, 112070M (2019).

Ultra-sensitive biosensor based on micro resonators

A micro-toroid is designed, capable of resolving the angular orientation of few-nanometer objects, applicable in fundamental life studies such as studying dynamics of a DNA strand.

$$\frac{\Delta\lambda_r}{\lambda_r} = \frac{W_P}{W_c} = \frac{\alpha|E_0(\mathbf{r}_P)|^2}{2\int \varepsilon(\mathbf{r}_c)|E_0(\mathbf{r}_c)|^2 dV_c}$$



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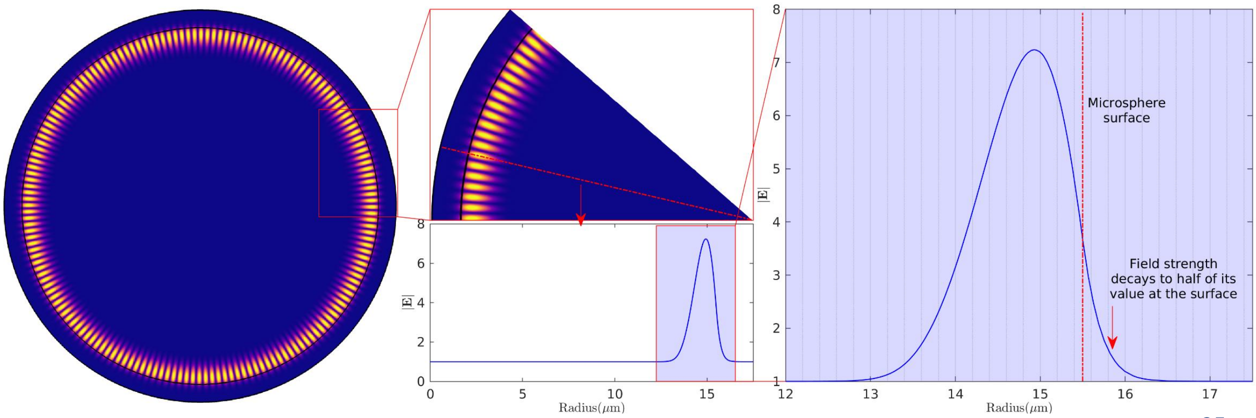

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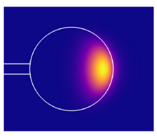
Ultra-sensitive biosensor based on micro resonators
Adding a thin dielectric shell:

- we propose adding a thin dielectric shell with refractive index close to the micro-resonator's refractive index in order to improve the resonator's quality factor through reducing the radiation loss.
- The challenge is the huge computational domain which should be explored in the Eigen-mode study.
- Using the azimuthal symmetry, only a cross section of the micro-toroid is simulated.

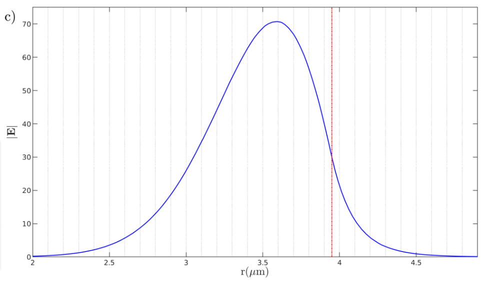
a)



b)

Resonance Frequency	353.2 THz
Quality Factor	5×10^{12}
Mode Volume	60.7 μm^3

c)



Ultra-sensitive biosensor based on micro resonators Adding a thin dielectric shell:

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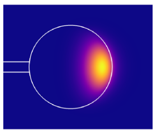

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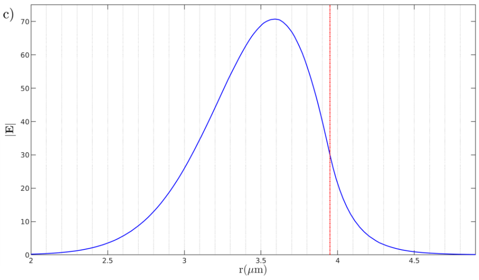
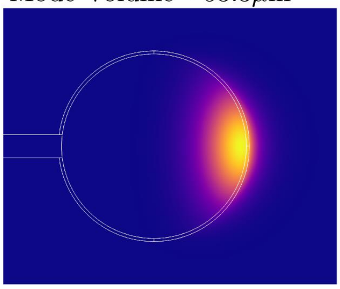
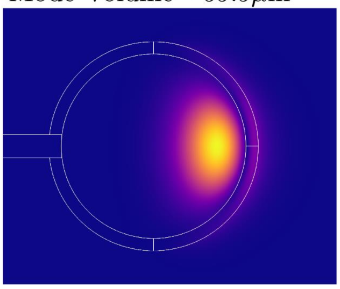


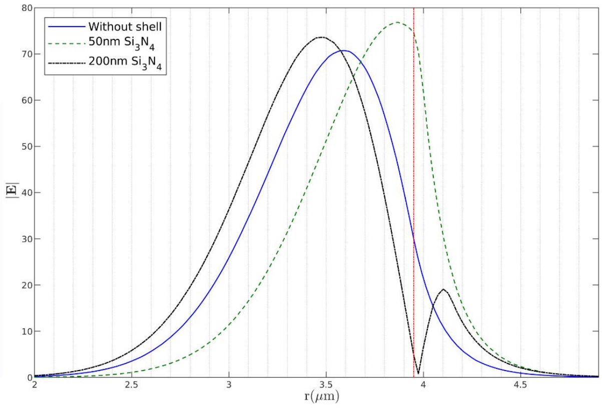
Si_3N_4 shell

50nm shell
$Q_F = 3 \times 10^{13}$
Mode-Volume= $53.3 \mu m^3$



200nm
$Q_F = 2.5 \times 10^{11}$
Mode-Volume= $59.9 \mu m^3$





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Universität Duisburg-Essen
Feb. 20th, 2020, Duisburg, Germany

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Thank you for your attention!