Heat released by plasmonic excitation of hybrid nanoparticles: effect on proton relaxation

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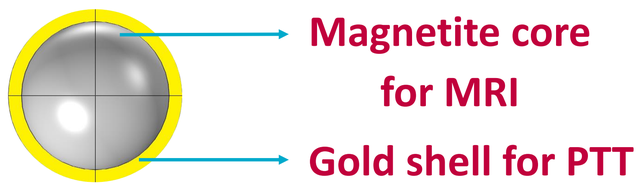
Abstract

Theranostics, which combines diagnosis and treatment in medicine, utilizes innovative hybrid nanoshells (NS) with gold plasmonic properties and magnetite cores. They enable simultaneous photothermal therapy (PTT) and magnetic resonance imaging (MRI). Our research investigates the temperature effects of photothermal therapy on the proton relaxation, in MRI, and optimizes nanoshell geometry for improved results, showing promise for biomedical applications.

Studied structure

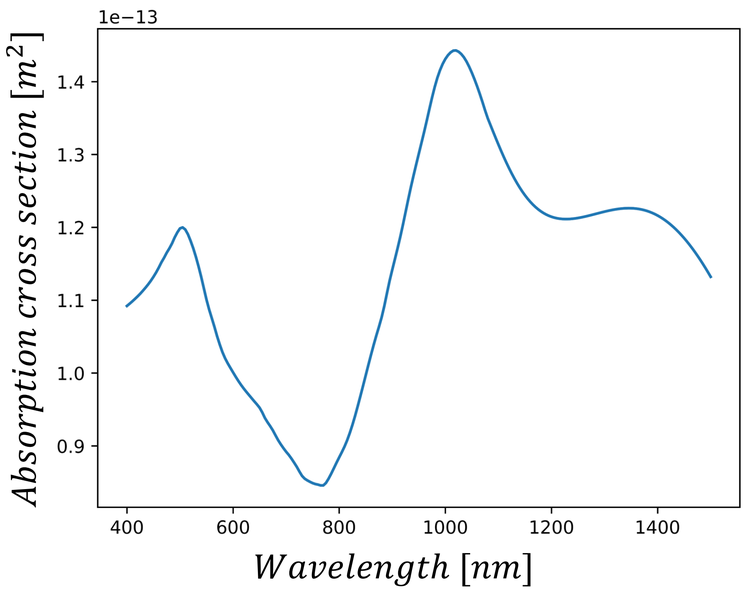
- Nanoshell: magnetite core + gold shell



- Allow photothermal therapy + MRI
- Occurrence of plasmonic hybridization between nanosphere/nanocavity

→ **multiple peaks in the absorption spectrum**

→ **high tunability to match biological window**

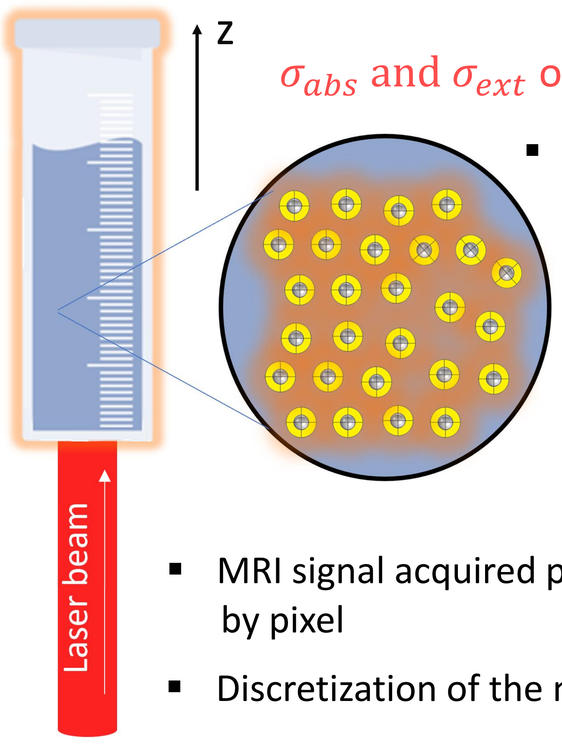


Heat rise mapping

- The collective thermal model [1] :

$$T_{collective}(\vec{r}) = \iiint_{Beam_{laser}} \frac{q(\vec{r'})}{4\pi\kappa_s |\vec{r'} - \vec{r}|} dr' \quad \text{with} \quad q(\vec{r'}) = I_0 \, N \, \sigma_{abs} \, e^{(-\sigma_{ext} N z)}$$

Heat power density; NP absorption cross section; Distance in sample; NP extinction cross section

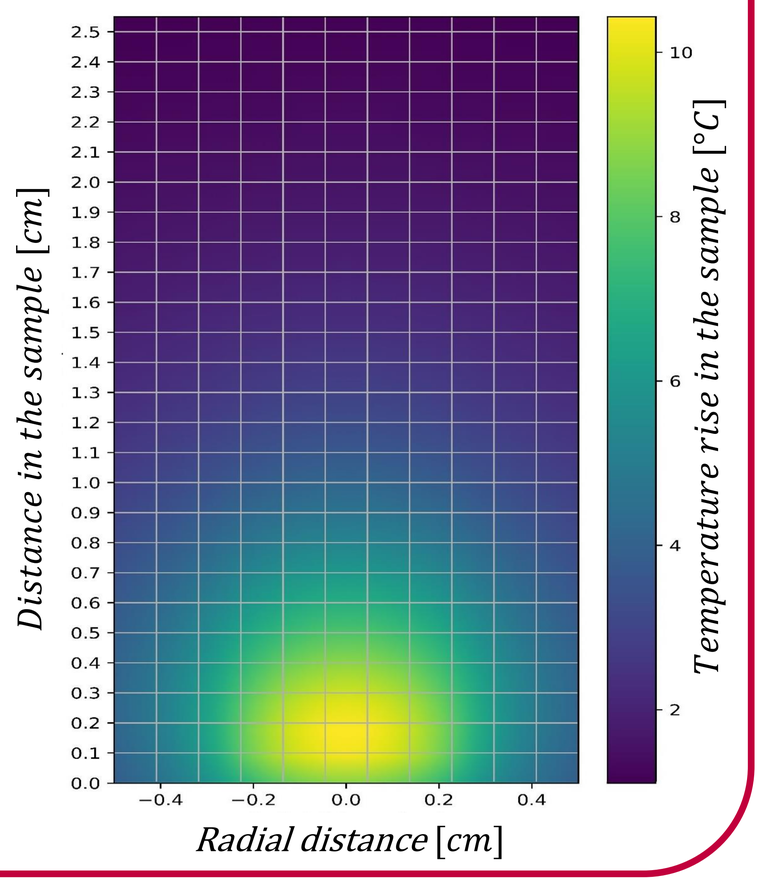


σ_{abs} and σ_{ext} obtained via COMSOL simulations

- Collective model used to map temperature change in the sample

- MRI signal acquired pixel by pixel
- Discretization of the map
- Need to obtain the average temperature of a pixel

We apply the appropriate theoretical MRI model to each pixel to map R_2

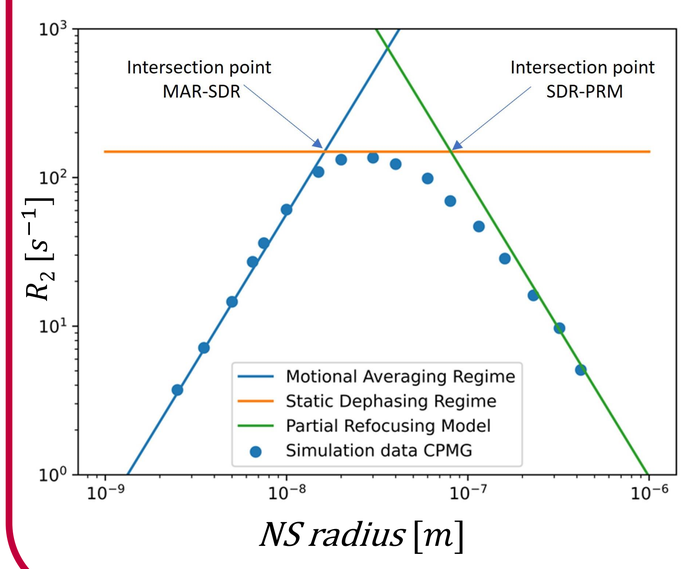


MRI models

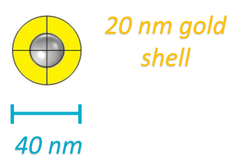
- Relaxation of the protons characterised by a relaxation rate
- Three different relaxation regimes:

→ **depending on NS size, water coefficient diffusion and saturation magnetization of the magnetite core**

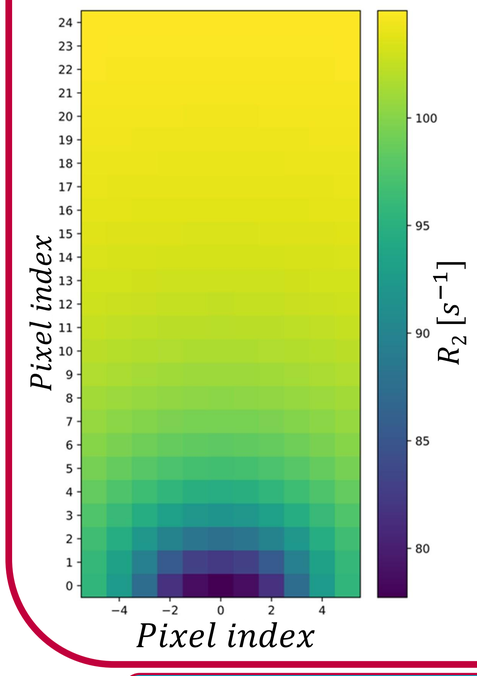
Model selection based on the intersection between models

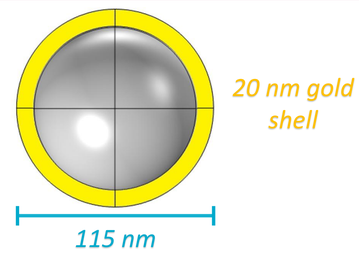


Results

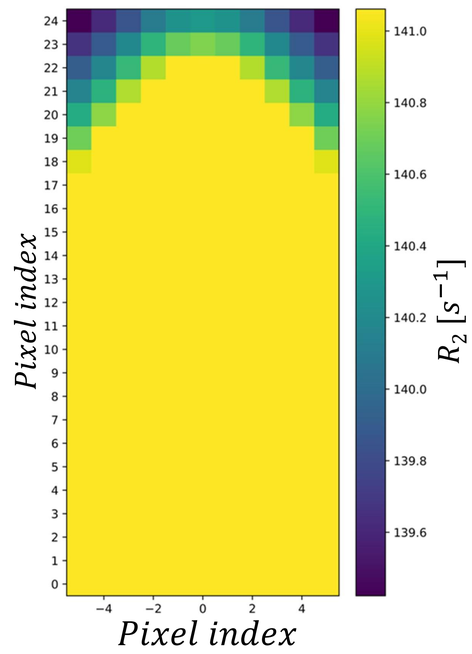


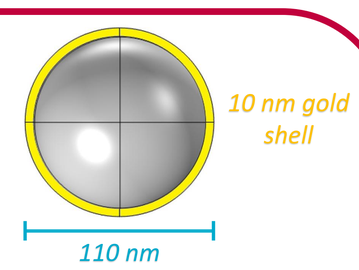
Plasmonic resonance → λ = 580 nm



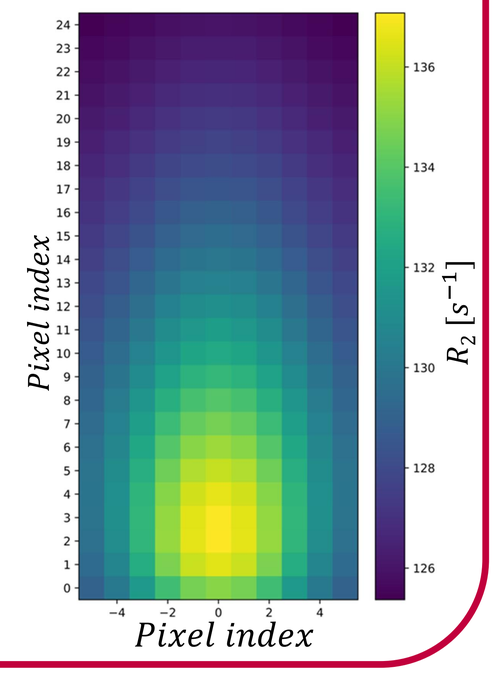


Plasmonic resonance → λ = 710 nm





Plasmonic resonance → λ = 870 nm



Conclusion

A small modification in the nanoshell's geometry can result in a significant change in the relaxation rate response!

[1] G. Baffou, Thermoplasmonics: Heating Metal Nanoparticles Using Light, Cambridge: Cambridge University Press, 2017.

[2] Q. L. Vuong et al., « Monte Carlo simulation and theory of proton NMR transverse relaxation induced by aggregation of magnetic particles used as MRI contrast agents », 2011.

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