Aggregation-Driven Effects of Hybrid Nanoparticles on Light Response, Heat Generation, and MRI Contrast

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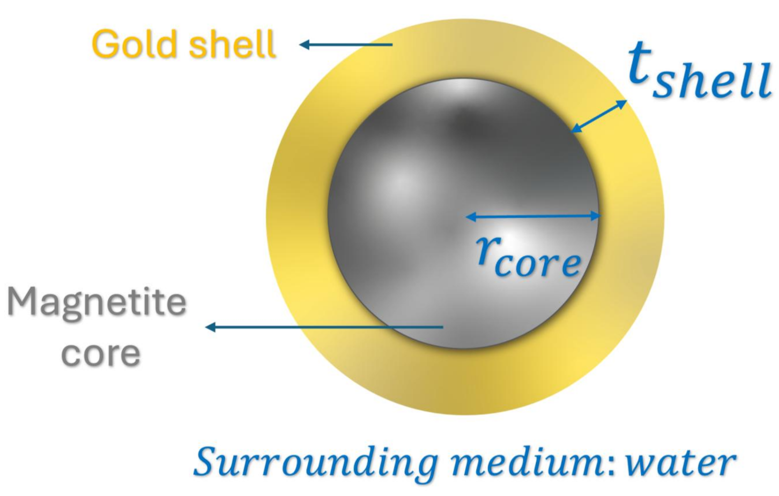
Abstract

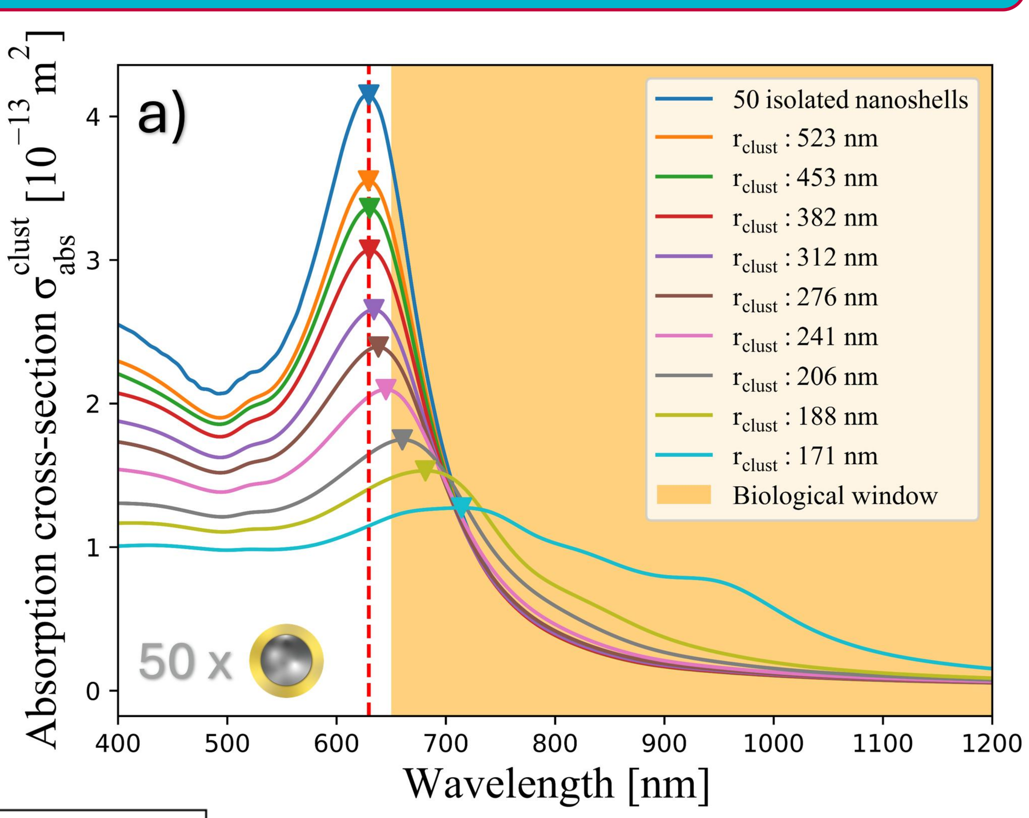


This work explores hybrid gold–magnetite nanoshells as theranostic agents for combined photothermal therapy and magnetic resonance imaging (MRI) under the clustering assumption. Finite element simulations characterize heat generation at the cluster scale, while a collective model predicts macroscopic temperature rise. An analytical theory calculates transverse relaxation rate (R_2) changes, considering aggregation and temperature effects. Aggregation enhances local heating but reduces overall temperature increase and R_2 contrast. Despite this, MRI can still distinguish dispersed from aggregated systems, highlighting the dual role of aggregation and the potential of hybrid nanoshells for non-invasive monitoring of laser-induced heating.

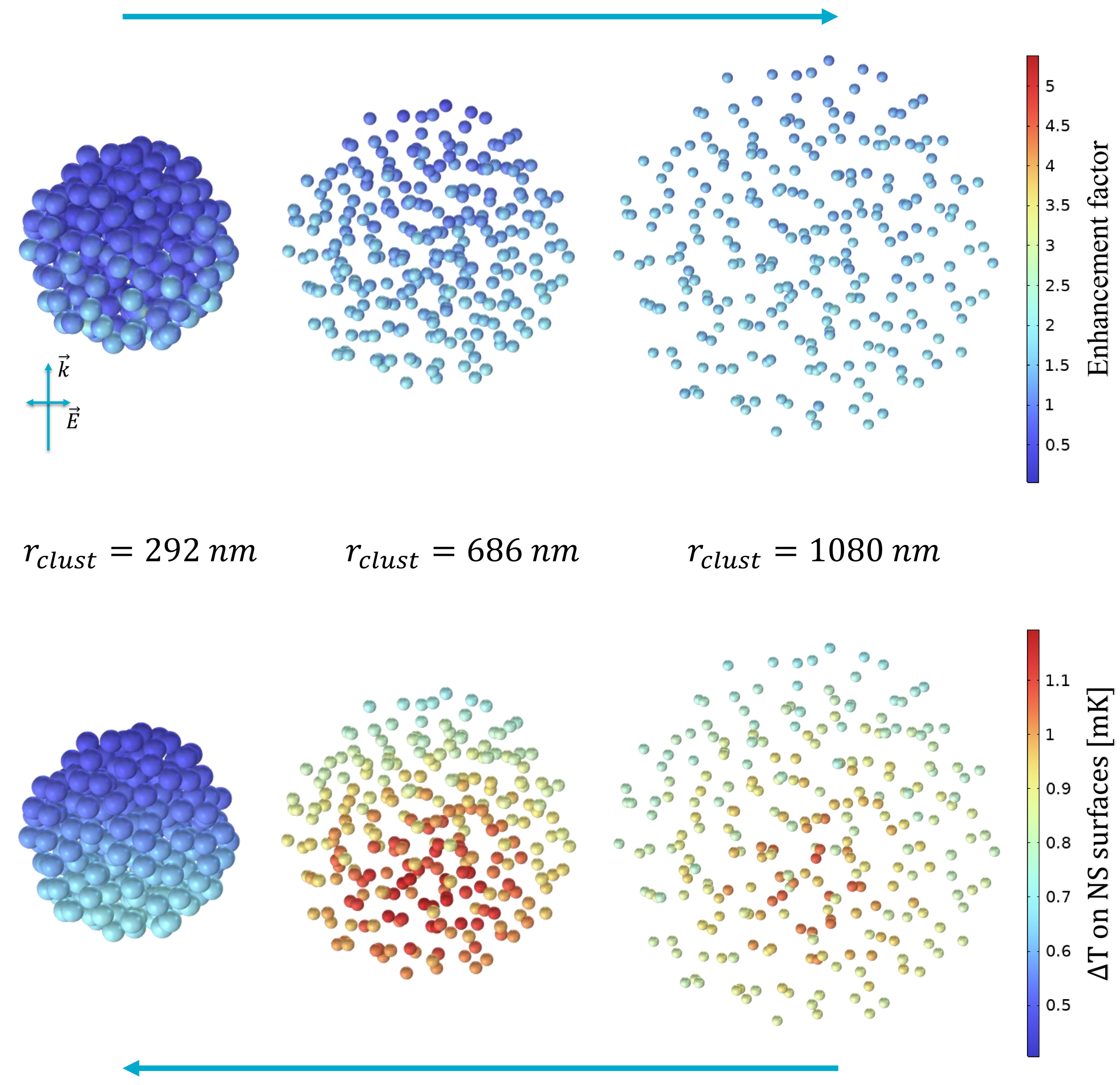
NS Cluster Local-Scale Thermoplasmonic Study

Transition between the independent scattering regime and the dependent one at a radius of about 350 nm

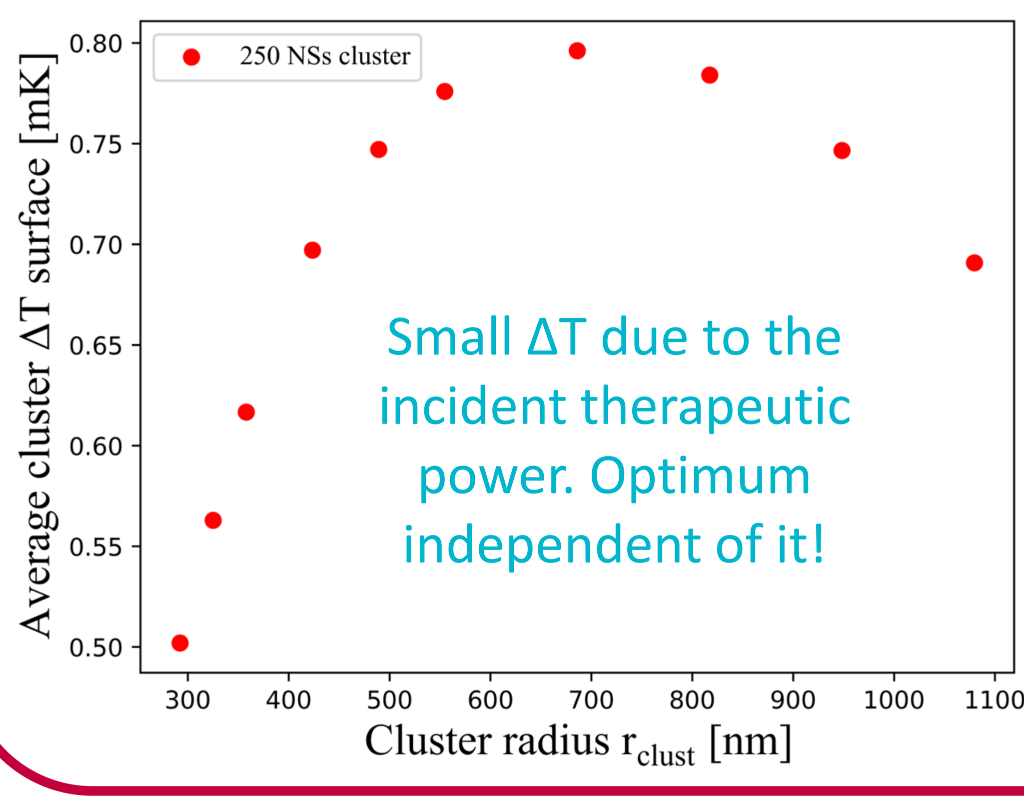
Appearance of a redshift in the absorption spectrum



Optical shielding ↘



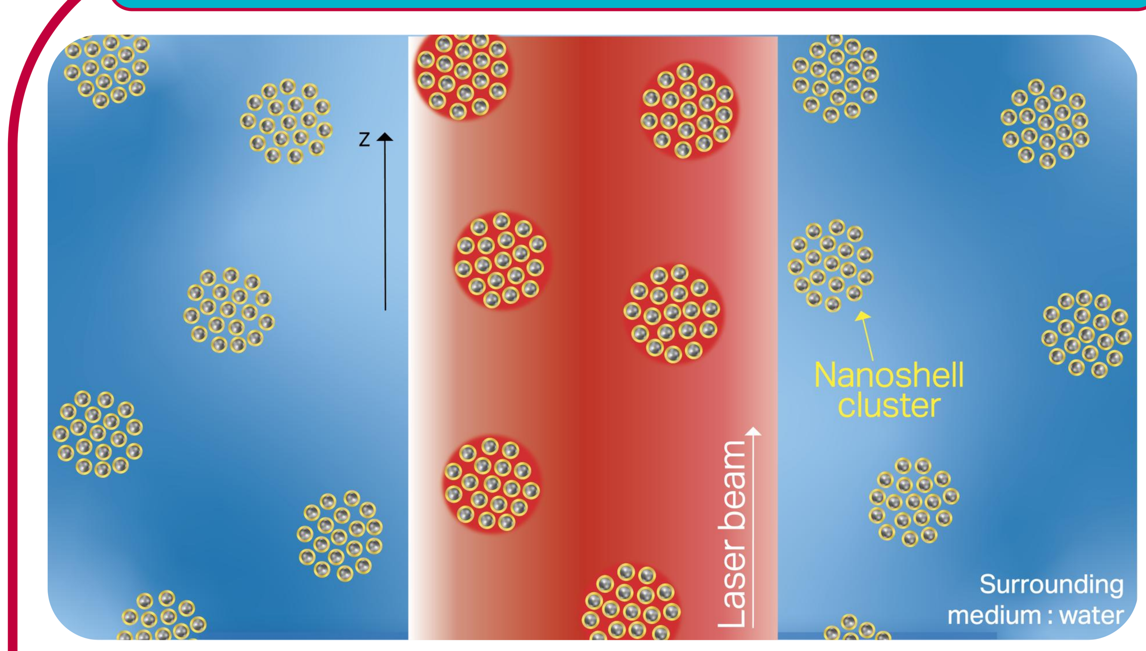
Thermal superposition effect ↗



Interplay between optical shielding and the thermal superposition effect

Existence of an optimum for the temperature rise at the cluster boundary as a function of the cluster radius/density

T°C rise at the macroscale



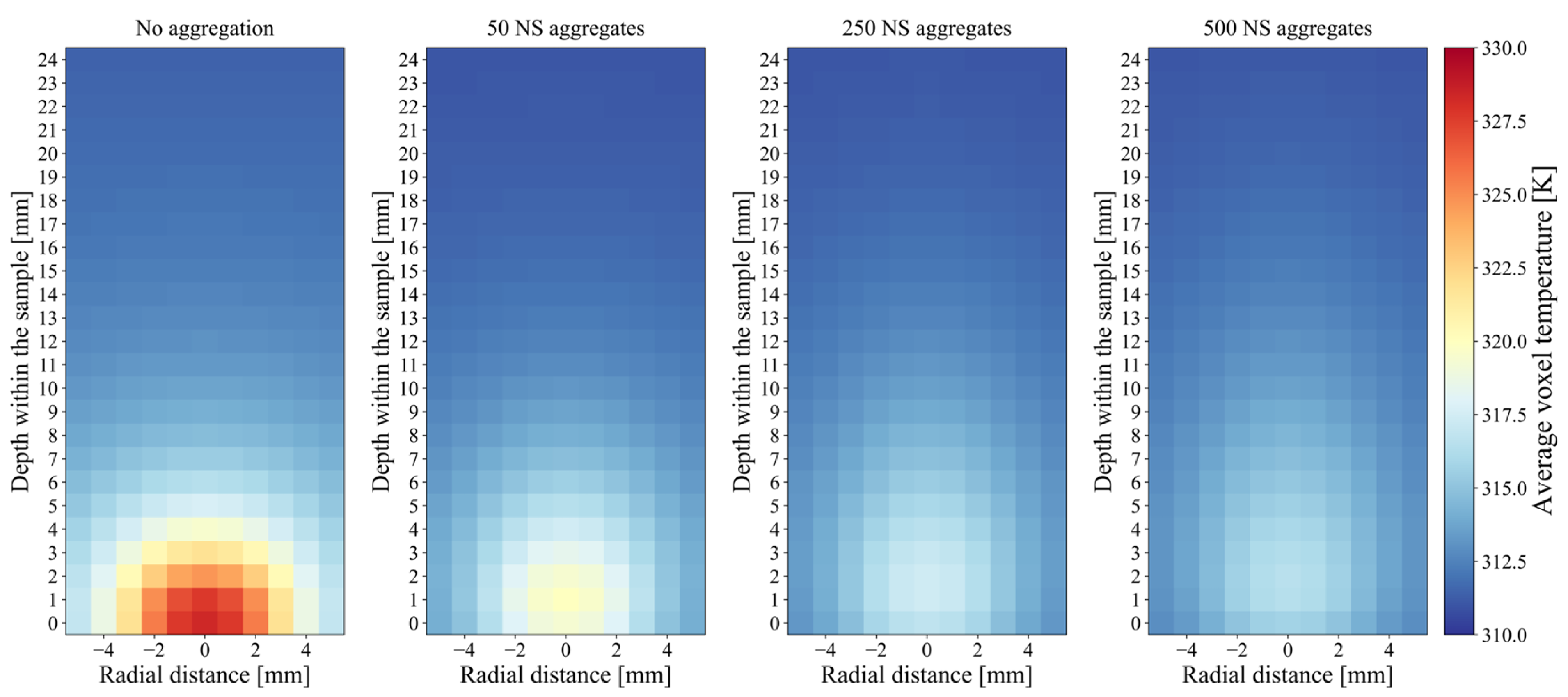
- The collective thermal model [1] :

$$T_{collective}(\vec{r}) = \iiint_{Beam_{laser}} \frac{q\left(\vec{r'}\right)}{4\pi\kappa_s\left|\vec{r'}-\vec{r}\right|}dr'$$

$$q\left(\vec{r'}\right) = I_0\ N\ \bar{\sigma}_{abs}\ e^{(-\bar{\sigma}_{ext} N\ z)}$$

Heat power density; Mean absorption cross-section of clusters; Mean extinction cross-section of clusters; Distance in sample

$\bar{\sigma}_{abs}$ and $\bar{\sigma}_{ext}$ obtained via averaged COMSOL simulations



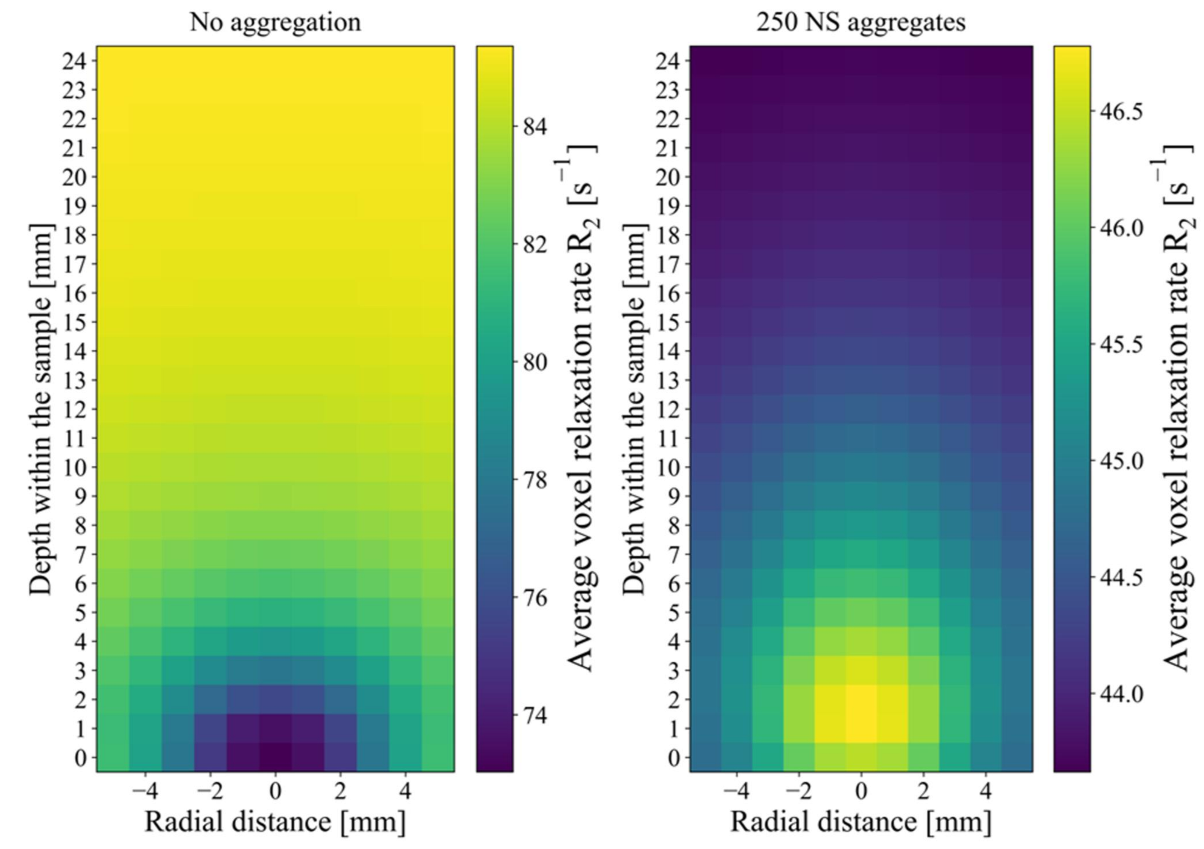
Fixed nanoshell concentration: 8,875 × 10^{16} NSs/m^3

The local optimum does not affect the macroscopic temperature rise.

Aggregation leads to a reduced temperature increase.

MRI contrast of clusters

- MRI contrast arises from differences in transverse and longitudinal proton relaxation.
  → Transverse proton relaxation characterized by the transverse relaxation rate (R_2)
- Transverse proton relaxation in magnetic particle cluster modeling [2]
  → In this work: adaptation of the model to account for temperature variations
- Application of the adapted relaxation model to previously obtained temperature maps:



Aggregation reduces the impact of temperature rise on R2. Strong dependence of R2 on the aggregation level

Potential to monitor phototherapy-induced cancer cell damage via NP aggregation tracking!

[1] G. Baffou, Thermoplasmonics: Heating Metal Nanoparticles Using Light, 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 », Journal of Magnetic Resonance (2011)

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We acknowledge support from the Action de Recherche Concertée (project ARC-23/27UMONS3)