

# *Solvent-dispersible nanostructured MIMI: an experimental and computational study*

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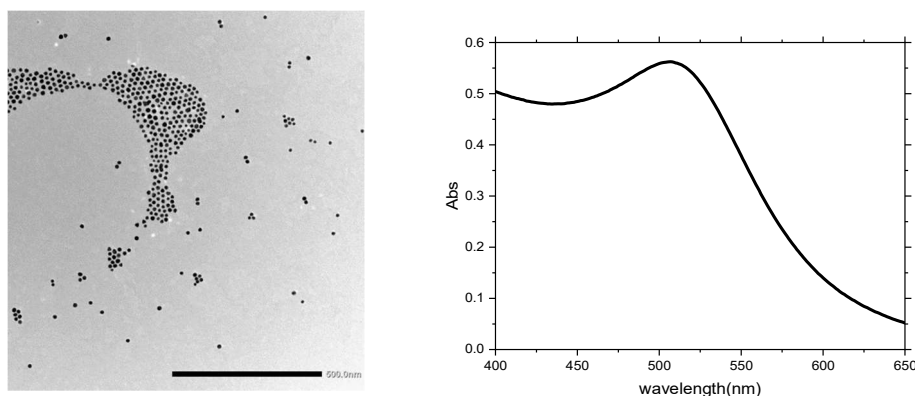


Figure S1. TEM images and Uv-vis spectra of AuNS@NaCit

## Cross-Section calculations

In electromagnetic scattering problems the total wave can be decomposed into incident ( $\mathbf{E}_{inc}$ ) and scattered waves ( $\mathbf{E}_{sc}$ ). From the scattered fields important physical quantities can be obtained as the cross section, which can be defined as the net rate at which electromagnetic energy ( $W$ ), crosses the surface of an imaginary sphere centered at the particle divided by the incident irradiation ( $\mathbf{P}_{inc}$ ) defined as:

$$\mathbf{P}_{inc} = \frac{1}{2\eta} |\mathbf{E}_{inc}|^2 \hat{\mathbf{k}} = \frac{1}{2} c\epsilon |\mathbf{E}_{inc}|^2 \hat{\mathbf{k}}$$

Where  $\eta$  is the characteristic impedance,  $\epsilon$  is the permittivity of the environment,  $c$  is the speed of light and  $\hat{\mathbf{k}}$  is the direction of the incident wave propagation.

The energy loss ( $Q_{loss}$ ) rate in a particle is:

$$Q_{loss} = \frac{1}{2} \text{Re}[\mathbf{J}_{tot} \cdot \mathbf{E}^* + j\omega \mathbf{B} \cdot \mathbf{H}^*]$$

Where  $\mathbf{J}_{tot}$  is a superposition of conduction and displacement currents.

The calculation of the cross sections, described in the main text, have been calculated for all the nano-objects (Figure S2).

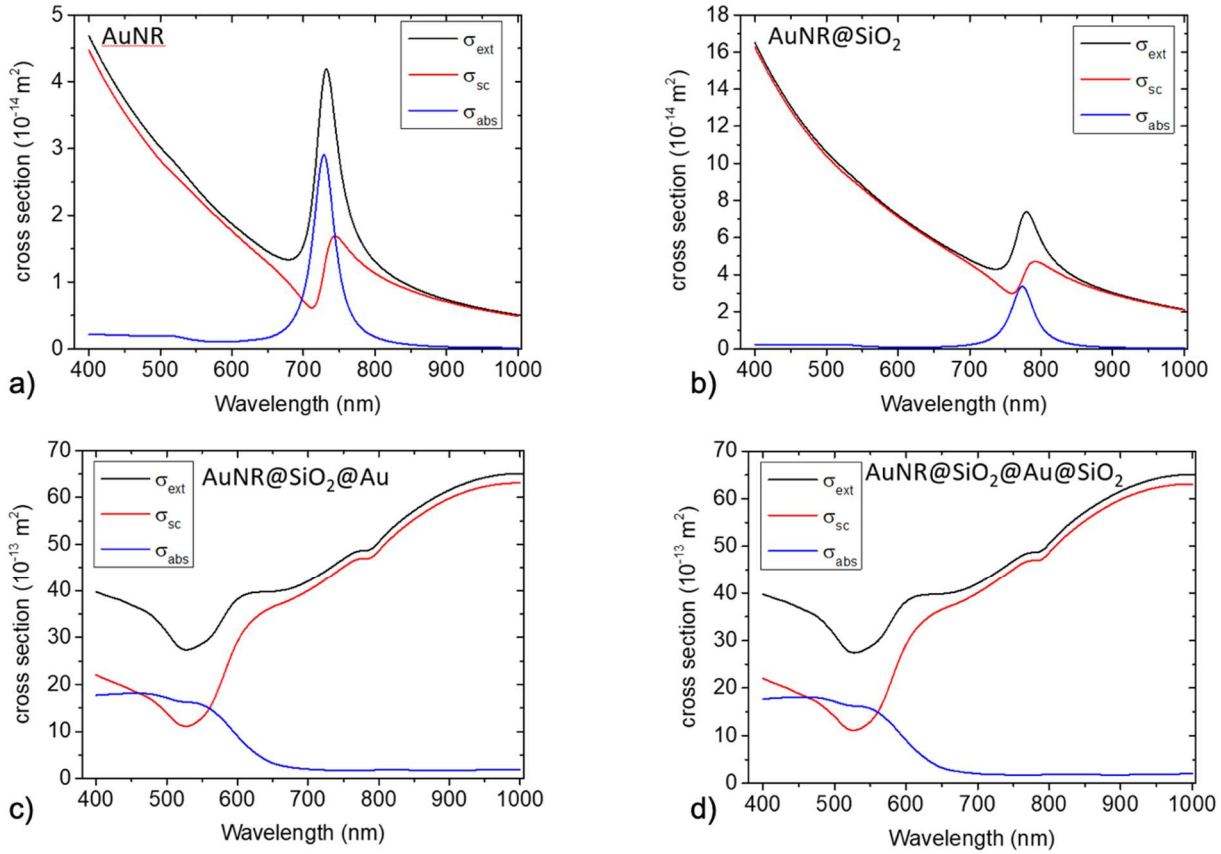


Figure S2. Calculated extinction, absorption and scattering cross sections of the (a) AuNR, (b) AuNR@SiO<sub>2</sub>, (c) AuNR@SiO<sub>2</sub>@Au and (d) AuNR@SiO<sub>2</sub>@Au@SiO<sub>2</sub>.

Quantity	Expression in Comsol	Value	Description
E0	3E5[V/m]	3E5 V/m	Electromagnetic Field
Radius	30[nm]	3E-8 m	Radius of the sphere
r_pml	Radius*8	2.4E-7 m	Radius of PML
t_pml	Radius*3	9E-8m	Thickness of PML
Lambda	515[nm]	5.15E-7 m	Wavelength
Frequency	C_const/Lambda	5.82E14 1/s	Frequency
Lambda_min	400[nm]	4E-7m	Minimum wavelength
Lambda_max	1000[nm]	1E-6m	Maximum wavelength
Lambda_step	5[nm]	5E-9m	Wavelength step
Sigma_geom	pi*(radius)^2	2.83E-15 m^2	Geometric cross section
S_in	E0^2/(2*Z0_const)	1.19E8 W/m^2	Scaling Factor
n_medium	1.333	1.333	Refractive index surrounding medium

Table S1. Parameters list used in the numerical modelling of the nanostructured.

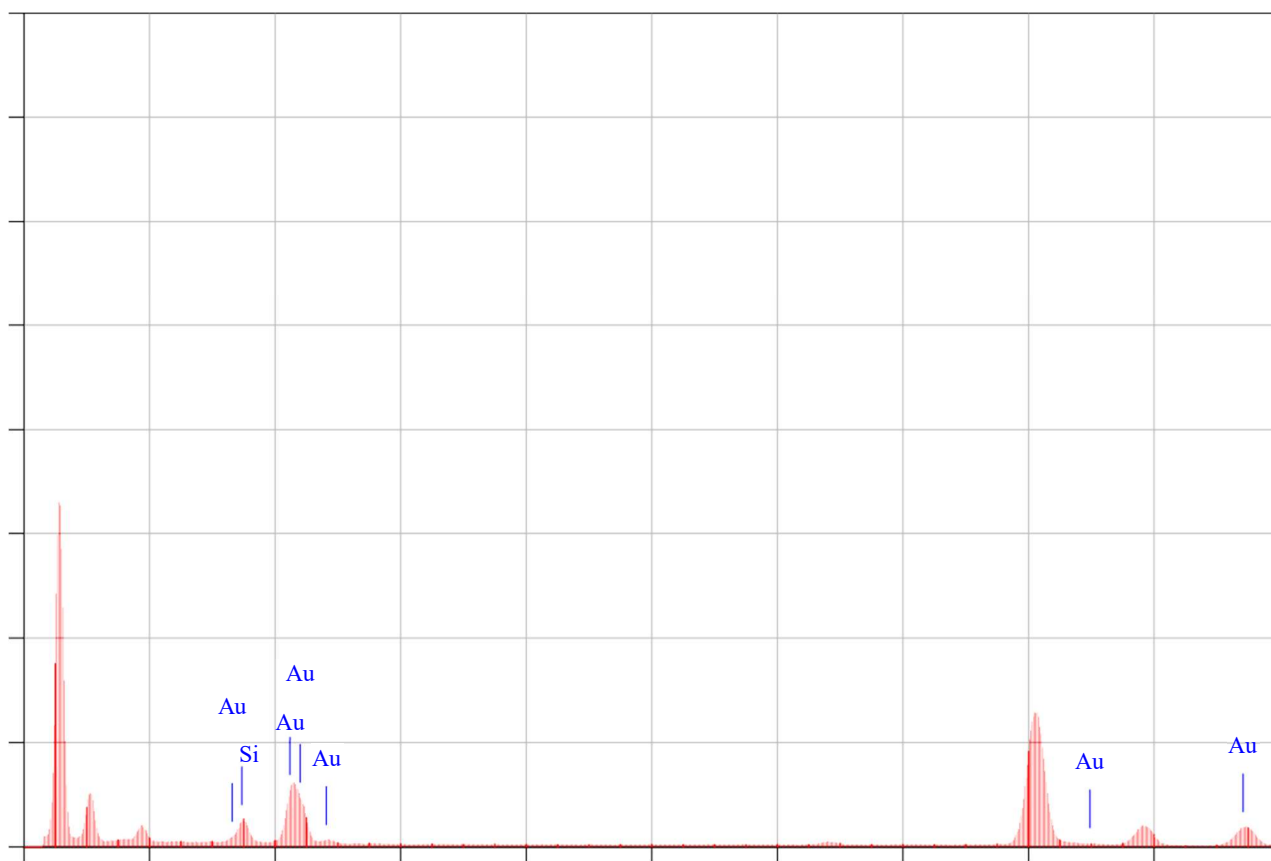


Figure S3. EDX measurement of AuNR@SiO<sub>2</sub>@Au@SiO<sub>2</sub>