Supporting Information:

Influence of Magnetic Field on the Two-Photon Absorption and Hyper-Rayleigh Scattering of Manganese-Zinc Ferrite Nanoparticles

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Materials and Methods

Structural characterization

Several experimental techniques can be used to determine structural parameters of nanostructures, as nanoparticles. Some examples are transmission electron microscopy (TEM), dynamic light scattering (DLS) and small-angle X-rays scattering (SAXS). Each one is sensitive to specific parameters and has advantages and disadvantages over the others. Dynamic light scattering is a technique that provides the distribution of the hydrodynamics radius of the nanoparticles, instead of the crystal size, since it is sensitive to fluctuations of the refractive index. On the present work, in which the NP’s optical properties are studied, the crystalline size is more important than the hydrodynamics radius, since the electrons are confined in this region. TEM and SAXS, on the other hand, are both sensitive to variations on the electronic density, thus providing information on the crystalline size of the nanoparticles. Nevertheless, the two techniques differ on the experimental procedure. Despite TEM being able to provide a direct image of the nanoparticles, it requires sample preparation as solvent evaporation, modifying the equilibrium condition of the system. Any aggregation of nanoparticles observed in TEM images is not clear to be present in solution or if it is only an artifact induced by the drying process. Besides, several pictures need to be taken for an adequate statistical analysis, but it is not guarantee that all the images are a proper representation of the system. Small-angle X-rays scattering, on the other hand, provides information on the reciprocal space about the NP’s structure. However, no special sample preparation is needed besides the transference to the proper vessel (in the present case, quartz capillaries). Therefore, structural parameters can be measured with nanoparticles in solution, and no artifacts are induced. The obtained results corresponds to a temporal and orientational average of the nanoparticles, ensuring a proper statistical analysis and that the system is well represented by the results. Furthermore, SAXS measurements can be performed in the presence of magnetic fields, allowing the verification of the formation
on chain-like structures. Since the obtained results are in the reciprocal space, a model is requested in order to obtain information about the size and shape of the nanoparticles.

**Hyper-Rayleigh Scattering**

An infra-red (IR) beam, $\lambda = 1064$ nm, was focused in the center of a square cuvette with length of 10 mm. The IR beam was emitted by a Q-switched and mode-locked (ML) laser (Nd:YAG from Coherent Inc., model Antares 76-S), generating around thirty ML pulses of 100 pico-second modulated by a Q-switched envelope of 150 ns FWMH. Since the nonlinear light scattering is isotropic on the plane of the optical table for a vertically polarized beam, a photo-multiplier tube (PMT) was used to detect the nonlinear light scattering in the orthogonal direction to the laser beam propagation, as illustrated on figure S1, with a band-pass filter centered on 532 nm ($F_{532}$) placed on its front, ensuring the detection of just the second-harmonic light. For that, a collimation system, lenses $L_2$ and $L_3$, was used to collect the scattered light and focalize it on the window of the photo-multiplier tube. Besides, in order to increase the signal-to-noise ratio, a spherical mirror (M) was added on the opposite direction to the PMT, with the center of curvature matching the focal point of the focusing lens ($L_1$) and the collimation lens to the detection system, $L_2$. The sample, the focusing and collimating lens, the spherical mirror and detector were placed inside a box of dimensions 50 cm $\times$ 30 cm $\times$ 30 cm to avoid light from other sources than the nonlinear process, while a low-pass filter ($F_L$) was placed in front of the only opening of the box in order to avoid any harmonics generated on other optical elements.

From the hyper-Rayleigh scattering experiment, the first-order hyperpolarizability $\beta$ can be determined by means of the equation

$$I (2\omega) = GN\beta^2 I^2 (\omega), \quad (S1)$$

in which $I (2\omega)$ is the total intensity of the scattered light, $I (\omega)$ the incident beam intensity,
Figure S1: Schematic representation of the hyper-Rayleigh scattering experimental setup. An infra-red beam was focused on the center of a squared cuvette by a convergent lens L₁ after entering a black box through a low-pass filter F₅₃₂. The nonlinear scattered light was collected and focalized on a photo-multiplier tube PMT by a set of lenses L₂ and L₃. In order to increase the signal-to-noise ratio a spherical mirror M was added to the opposite direction of the PMT. To guarantee the detection of the second harmonic only, a band-pass filter F₅₃₂ centered on 532 nm, the half of the wavelength of the incident beam, was placed in front of the detector.

N the number of scattering units per unity of volume and G an experimental factor related to geometrical parameters and detectors efficiency, among others. In the current experimental setup there is no need of elements to change the incident intensity \( I(\omega) \) due to the Q-switch envelope that imposes different intensities for the mode-locked pulses, that is, with a single pulse train different values of the incident and scattered intensities are verified.

The harmonic generation occurs around the focal region, due to high electric fields, and the scattered light must travel within the sample in order to reach the detector. If losses in the second harmonic are present due to absorption or scattering, the intensity of the detected signal \( S(2\omega) \) is smaller than the intensity of the scattered radiation \( I(2\omega) \) and therefore must be corrected taking into account the light attenuation \( A(2\omega) \). Thus, when the focal point corresponds to the center of the cuvette and considering the spherical mirror, the total scattered intensity is:

\[
I(2\omega) = \frac{2S(2\omega)}{10^{-\frac{1}{2}A(2\omega)} + 10^{-\frac{3}{2}A(2\omega)}}. \tag{S2}
\]
To properly determine the hyperpolarizability $\beta$ from the equation S1, the external reference method\(^3\) (ERM) was used. In this case, the scattering amplitude is measured for the sample in different concentrations of scattering units N. Since the quadratic coefficient $Q = I(2\omega)/I(\omega)$ depends linearly on N, the proportionality constant $a_{\text{sample}} = G\beta^2_{\text{sample}}$ can be calculated. Then, without changing the experimental conditions, the scattering from a standard material (ref), with hyperpolarizability $\beta_{\text{ref}}$ well defined, is measured also in different concentrations and the parameter $a_{\text{ref}} = G\beta^2_{\text{ref}}$ is determined. As the experimental conditions remained unchanged, the experimental parameter G in the two measurement processes, sample and reference, is the same and, therefore, the sample first-order hyperpolarizability can be determined as:\(^4\)

$$
\beta_{\text{sample}} = \beta_{\text{ref}} \sqrt{\frac{a_{\text{sample}}}{a_{\text{ref}}}}. \quad (S3)
$$

**Nonlinear absorption**

An infra-red beam with Gaussian profile and wavelength 800 nm was obtained from an Astrella amplifier system, Coherent Inc., emitting 80 fs pulses at the laser exit with repetition rate of 100 Hz, in order to avoid thermal effects\(^5,6\) on the sample. As presented on S2, the beam was focused by a lens $L_1$, with focal length of 200 mm, while the sample was positioned in a motorized station and translated around the focal point. The studied colloidal dispersions were allocated on a sample holder composed of two pieces of microscope slide and a 200 $\mu$m thick Teflon spacer. The total light transmitted through the sample was collected by a second convergent lens $L_2$ and focused on a fast photodetector (Thorlabs SV2-FC), while the transmittance through the sample for each position in the beam path was registered.

The absorption coefficient $\alpha$ of a material in the presence of a high intensity light, as the one originated from a femtosecond pulsed laser, depends on the incident intensity\(^7\) $I$
Figure S2: Illustration of the Z-Scan experimental setup. An infra-red beam was focused by a convergent lens $L_1$ and the sample translated around the focal position. In order to determine the nonlinear absorption coefficient, a second lens $L_2$ was used to collect all the transmitted light and focus it on the window of a fast photodetector. Since all the light passing through the sample was collected, the ZS experiment in the open-aperture configuration was sensible to nonlinear absorption.

According to:

$$\alpha = \alpha_0 + \alpha_{2PA} I$$  \hspace{1cm} (S4)

in which $\alpha_0$ is the linear absorption coefficient and $\alpha_{2PA}$ is the two-photon absorption coefficient. On the Z-Scan technique, the transmittance by the sample at any position $z$ is normalized by the transmittance at a position far from the focus $z_F$, where nonlinear effects are not present. Therefore, variations on the normalized transmittance $T_N(z) = T(z)/T(z_F)$ are only due to nonlinear effects, specifically two-photon absorption in the present case. In order to determine the 2PA coefficient from the normalized transmittance curves obtained in the ZS experiment, the Sheik-Bahae model $^8$ for the open-aperture case was used and is given by:

$$T_N(z) = \frac{1}{\sqrt{\pi q_0(z, 0)}} \int_{-\infty}^{\infty} \ln \left[ 1 + q_0(z, 0) \exp \left( -\tau^2 \right) \right] d\tau,$$  \hspace{1cm} (S5)

in which $q_0(z, 0) = \frac{\alpha_{2PA} I_0 L_{eff}}{1 + (z/z_0)^2}$, with $I_0$ the on axis intensity at the focus, $L_{eff} = (1 - e^{\alpha_0 l})/\alpha_0$ is the effective sample thickness and $z_0$ the Rayleigh length.

A piece of quartz was used as a reference sample in order to determine the Rayleigh length as $z_0 = 1.5 \pm 0.2$ mm, thus the beam waist $w_0 = 20 \pm 2$ $\mu$m, and the experiments were performed with $I_0$ on the order of 80 W/cm$^2$. Due to the small thickness of the samples, the experiments were performed with the MZS samples at the concentration of $9.3 \times 10^{19}$.
units/cm$^3$ and the MZC, $4.3 \times 10^{19}$ units/cm$^3$. The two-photon absorption cross-section$^{10}$ $\sigma_{2PA}$ was then calculated as:

$$\sigma_{2PA} = \frac{h\nu}{N^{\alpha_{2PA}}} ,$$

(S6)

in which $h\nu$ is the energy of the incident photon and $N$ the concentration of $\text{Mn}_{0.5}\text{Zn}_{0.5}\text{Fe}_2\text{O}_4$ units, allowing the results comparison for the two samples measured in different concentrations, as well as with other systems.

**Results**

**Structural characterization**

In the present case, nanoparticle’s structural characterization was carried out by the small angle x-rays scattering without external magnetic fields, enabling the NPs shape and size determination. From the isotropic 2D scattering pattern measured by the detector, a unidimensional curve of scattering intensity as a function of the scattering vector modulus $q = \frac{4\pi \sin \theta}{\lambda}$ ($2\theta$ is the scattering angle and $\lambda$ the wavelength) was obtained integrating the experimental result on the azimuthal angle $\phi$, on the plane of the image.

The x-rays scattering intensity was modeled as a collection of NPs of a given shape and size polydispersity. For the present case, the intensity is given by:

$$I_{\text{par}}(q) = \int_0^\infty D(r)V(r)^2 P(q, r) \, dr ,$$

(S7)

where $D(r)$ is a Gaussian function which represent a number size distribution centered in $R_0$ with standard deviation $\sigma$, $V(r)$ the volume of a particle with characteristic dimension $r$ and $P(q, r)$ the form factor of the particle for a given characteristic dimension $r$. The size distribution of the present magnetic nanoparticles was verified to be very narrow and because of that the Gaussian function was used, despite the fact that usually the size distribution of ferrofluid nanoparticles are associated with a lognormal distribution, since for small variances
\( \sigma^2 \) the two functions are comparable.

The modeled particles are created by the use of random points inside of a given shape. The MNPs shapes were built applying the following restrictions simultaneously:

\[
\begin{aligned}
|x| &< r \\
|y| &< r \\
|z| &< r \\
\sqrt{x^2 + y^2 + z^2} &< S_c \sqrt{3} r
\end{aligned}
\]

where, \( S_c \) is a parameter related to the NP shape and \( r \) is the characteristic dimension, that is, the radius of the sphere or half of the side of the cube. If \( S_c = 1 \), the NP is a cube with half sides \( r \), while if \( 1/\sqrt{3} < S_c < 1 \) it is a cube with rounded vertices, and if \( S_c = 1/\sqrt{3} \) it is a sphere with radius \( r \). For each shape, a surrounding layer of constant thickness \( t \) and relative electronic density \( \rho_{\text{out}} \) is included, representing the surfactant oleic acid molecules. The electronic density of the NP core is fixed equal \( \rho_{\text{shell}} = 1.0 \) while \( S_c, t \) and \( \rho_{\text{out}} \) are structural parameters optimized by fitting to experimental data, together with size polydispersity parameters \( r \) and \( \sigma \). By using the Monte Carlo method\(^{11,12} \) the intensity form factor is calculated.

Thus, the experimental data of scattering intensity for both MZS and MZC samples in the absence of magnetic field are shown on figure S3, as well as the correspondent fitting of equation S7. The unidimensional curves were obtained by azimuthal integration of the isotropic 2D scattering pattern. These curves were used to adjust the structural parameters for the spheres and cubes, that is, \( R, \sigma, S_c, t, \) and \( \rho_{\text{out}} \). For MZS samples was fixed \( S_c = 1/\sqrt{3} = 0.58 \), the size parameters were obtained as the radius of the sphere \( R = 66.0 \pm 0.2 \) Å and the relative standard deviation \( \sigma_{\text{Rel}} = \sigma/R_0 = 0.23 \pm 0.01 \), while the surfactant parameters \( t = 4 \pm 1 \) Å and \( \rho_{\text{out}} = 0.3 \pm 0.1 \). On the other hand, the fitting results for MZC samples were \( S_c = 0.78 \pm 0.01 \), in the range \( 1/\sqrt{3} < S_c < 1 \), which means the nanoparticle’s shape corresponds to a cube with rounded vertices. The characteristic dimension, the half
of the cube size, \( R = 48 \pm 6 \text{Å} \) and the relative distribution width \( \sigma_{\text{Rel}} = 0.32 \pm 0.01 \), while the surrounding layer parameters \( t = 8 \pm 2 \text{Å} \) and \( \rho_{\text{out}} = 0.4 \pm 0.1 \).

![Figure S3: Scattering intensity \( I(q) \) as a function of the modulus of scattering vector \( q \) for MZS (○) and MZC (□) samples in the absence of external magnetic field and the correspondent fit. Data was obtained integrating the isotropic 2D SAXS pattern.](image)

The form factor \( P(r, q) \) was calculated by the Monte Carlo method,\(^{11,12}\) using a random distribution of spherical subunits inside of a given shape, with the restrictions given by equation S8. From the fitting of eq. S7 to the experimental results shown on figure S3, the nanoparticles’ shape were constructed and are presented on figure S4, for the MZS (left) and MZC (right) samples, which allows the verification of the spherical shape of MZS samples and the cubic shape with rounded vertices of MZC ones. The model used in this work has been tested before, studying the clustering of low-density lipoproteins induced by heating,\(^{13}\) the oxidation of low- and high-density lipoproteins\(^{14}\) and the size and shape of magnetic nanoparticles,\(^{15}\) in which the obtained results were in agreement with transmission electron microscopy. Therefore, the performed SAXS measurements corresponds to a proper characterization of magnetic nanoparticles, specially with regard the crystalline size and morphology.
Therefore, the model fitted to small angle x-rays scattering results have shown that MZS nanoparticles presents spherical shapes with mean diameter of $13.2 \pm 0.4$ nm while the MZC NPs corresponds to cubes with rounded vertices and the characteristic cube size is $10 \pm 1$ nm. On this text, for simplicity, MZS and MZC samples are also called spherical and cubic nanoparticles.

**Linear attenuation**

The attenuation spectra for the MZC cubic nanoparticles is shown on figure S5 for wavelengths between 550 nm and 1000 nm. Measurements were performed for the solution in a sample holder of length $l = 200$ $\mu$m and at the concentration of $4.3 \times 10^{19}$ ferrite units/cm$^3$. Since the light source provides unpolarized radiation from halogen lamps, a calcite polarizer (Thorlabs GL-10, uncoated) was used to polarize the light first in the vertical then in the horizontal directions, while external magnetic field was applied in the horizontal direction. Therefore, on figure S5 is presented the attenuation spectrum for the solution in the absence of field and for the maximum applied field, $H = 3100$ Oe, both in the case where the field lines was parallel to the light polarization and in the perpendicular configuration. Since the results for the MZS solutions are analogous, they are not presented here.

Furthermore, it is shown on figures S6(a) and (b) the attenuation spectra of MZS and
Figure S5: Attenuation spectrum for cubic nanoparticles MZC in the absence and in the presence of magnetic field of magnitude $H = 3100$ Oe. The continuous line corresponds to the measurements performed in the absence of external field, while the dashed line corresponds to the results obtained with the light polarization parallel to the magnetic field lines. On the other hand, the dotted line was obtained with the light polarization parallel to the field.

MZC samples, respectively, for different concentrations. On figure S6(c) it is presented the optical density at 532 nm of the samples as a function of the concentration of ferrite units, in which the optical density presents a linear dependency on the concentration of Mn$_{0.5}$Zn$_{0.5}$Fe$_2$O$_4$ units. Since both samples are made from the same material, presenting differences only on size and shape of nanoparticles, the linear absorption must be the same when normalizing results by the basic units of interaction between light and matter, as was verified and shown on figure S6. Thus, a single linear fit was performed to experimental data from spherical and cubic nanoparticles and was used to calculate the losses during the HRS experiments for all the concentrations.

**Transient absorption**

On figure S7 is shown the temporal dynamics of the light absorbance from MZC nanoparticles, with temporal resolution of 100 fs. The x-axis shows the time delay between the pump and the probe pulses, the y-axis the wavelength while the color scale the absorbance.
Figure S6: Attenuation spectrum as a function of sample concentration for (a) MZS nanoparticles and (b) MZC ones. (c) Linear attenuation of light with wavelength 532 nm for samples containing spherical (●) and cubic (■) nanoparticles. A linear dependency was fitted for all experimental data since the constituents of both NPs are the same.

$$\Delta A = -\log_{10}(T_N).$$ For negative times observed on figure S7, the pump pulse hits the sample after the probe, thus $\Delta A = 0$. It can be observed that this region shifts for greater values of $t$ as the wavelength increases, which is a signature of the pulse chirp. When the probe beam optical path is increased and it illuminates the sample after the pump pulse, an increase in the absorbance is observed, correspondent to the excited state absorbance (ESA), which decays fast, but does not returns to $\Delta A = 0$ in the studied time range.

Similarly, the absorbance temporal dynamics with the maximum probe delay of 100 ps and temporal resolution of 1 ps is presented on figure S8. In this case, the fast response can be seen after the sample is illuminated by the pump beam and the offset persists for the measured time, indicating a much slower process.

In order to emphasize the time evolution, the change in the absorption $\Delta A = -\log_{10}(T_N)$
Figure S7: Time evolution of the absorbance $\Delta A = -\log_{10}(T_N)$ by MZC nanoparticles for wavelengths between 470 nm and 680 nm. Experiments were performed with temporal resolution of 100 fs.

for the wavelength $\lambda = 560$ nm is shown on figure S9(a) and S9(b) for MZS and MZC nanoparticles, respectively, for measurements performed with the maximum probe delay 100 ps and resolution of 1 ps. The fast decay observed for measurements in the 10 ps time scale is represented on the plots by a few experimental points of higher absorption, and the offset plateau fitted on that measurements is also observed here, unchanged in this time scale within the experimental errors, indicating even slower relaxation process.
Figure S8: Time evolution of the absorbance \( \Delta A = -\log_{10}(T_N) \) by MZC nanoparticles for wavelengths between 470 nm and 680 nm. Experiments were performed with temporal resolution of 1 ps.

Figure S9: Time dependent excited state absorption for MZS (a) and MZC (b) nanoparticles for the wavelength of 560 nm.
Small angle X-rays scattering

2D scattering pattern of MZS samples for $H = 0$ Oe and $H = 3200$ Oe is presented on figure S10. The scattering pattern without magnetic field, figure S10(a), is isotropic and corresponds to an temporal and orientational average of nanoparticles in solution. On the other hand, when the magnetic field is applied the SAXS pattern, represented on figure S10(b), becomes anisotropic since elongated structures are formed on the solution.

![Figure S10: 2D SAXS pattern of MZS magnetic nanoparticles in colloidal solutions in the absence of magnetic field (a) and with applied magnetic field of magnitude 3200 Oe in the horizontal direction. The horizontal black stripe on both figures is a blind region of the detector and is disconsidered during the data analysis.](image)

In figure S11 a simulation is shown with increasing values of the radius of gyration $R_G$ of aggregates. As one can clearly see, for sizes larger than 30 nm all information related to the aggregate size is not visible for $q$ values larger than 0.13 nm$^{-1}$, the minimum value for the scattering vector in our experiments.
Figure S11: Simulation of equation 1 with typical values for the particle size and $S_{HS}(q)$ interaction, with variable $R_G$ for the aggregate. The vertical dotted line indicates the $q_{\text{min}}$ accessible on our experiments.

The fitting of the experimental data obtained from the small angle X-rays scattering of spherical (MZS) and cubic (MZA) nanoparticles are presented on Table S1 for the horizontal and vertical cuts.
Table S1: Fitting parameters resultant from SAXS data analysis for MZS and MZC samples. The form parameter $S_c = 0.58$ for spheres and $S_c = 0.78 \pm 0.01$ for cubic nanoparticles and the surfactant parameters $t = 4 \pm 1 \, \text{Å}$ and $\rho_{out} = 0.3 \pm 0.1$ for MZS, and for MZC, $t = 8 \pm 2 \, \text{Å}$ and $\rho_{out} = 0.4 \pm 0.1$ were kept constant. The presented uncertainty corresponds to the standard error.

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References


