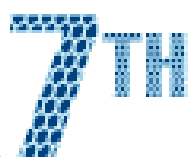




3NANO
2024
SCIENCE
TECHNOLOGY
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7TH

International Conference on Nanoscience,
Nanotechnology and Nanobiotechnology



**Abstracts
Book**



UNIVERSIDADE DE BRASÍLIA
Centro Internacional de Física da Matéria Condensada

**7th International Conference on Nanoscience,
Nanotechnology and Nanobiotechnology
Brasília, 26th – 29th November**

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TUE 26/11	WED 27/11	THU 28/11	FRI 29/11
	9:00 IT 6 <i>A. M. Figueiredo</i> 09:30 OC 1 <i>T. Fiuzza</i> 09:45 OC 2 <i>C. M. Ferreira</i> 10:00 IT 7 <i>N. Serradji</i> Chairperson: <i>J. Geshev</i>	9:00 IT 13 <i>N. Tomazio</i> 09:30 OC 3 <i>C. A. M. Vieira</i> 09:45 OC 4 <i>V. Cerqueira</i> 10:00 IT 14 <i>J. Geshev</i> Chairperson: <i>A. López-Ortega</i>	09:00 – 10:30 Collaborations and Discussions
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	11:00 IT 8 <i>F. Messina</i> 11:30 IT 9 <i>M. H. Sousa</i> Chairperson: <i>A. Campos</i>	11:00 IT 15 <i>C. Graeff</i> 11:30 IT 16 <i>L. Wouk</i> Chairperson: <i>A. M. Figueiredo</i>	11:00 IT 22 <i>E. Winkler</i> 11:30 OC 5 <i>F. G. Silva</i> 11:45 OC 6 <i>M. Baricic</i> 12:00 IT 23 <i>M. Vasilakaki</i> Chairperson: <i>J. Depeyrot</i>
13:00 Registration 14:15 Opening Ceremony	12:00 – 14:30 Lunch		12:30 Award and Closing Session
15:00 IT 1 <i>S. Ammar-Merah</i> 15:30 IT 2 <i>N.-T. Ha-Duong</i> 16:00 IT 3 <i>D. Muraca</i> Chairperson: <i>R. Aquino</i>	14:30 IT 10 <i>L. Paterno</i> 15:00 IT 11 <i>F. Silly</i> 15:30 IT 12 <i>E. Lima</i> Chairperson: <i>F. Messina</i>	14:30 IT 17 <i>J. J. Bonvent</i> 15:00 IT 18 <i>A. López-Ortega</i> 15:30 IT 19 <i>G. Gomide</i> Chairperson: <i>S. Ammar-Merah</i>	
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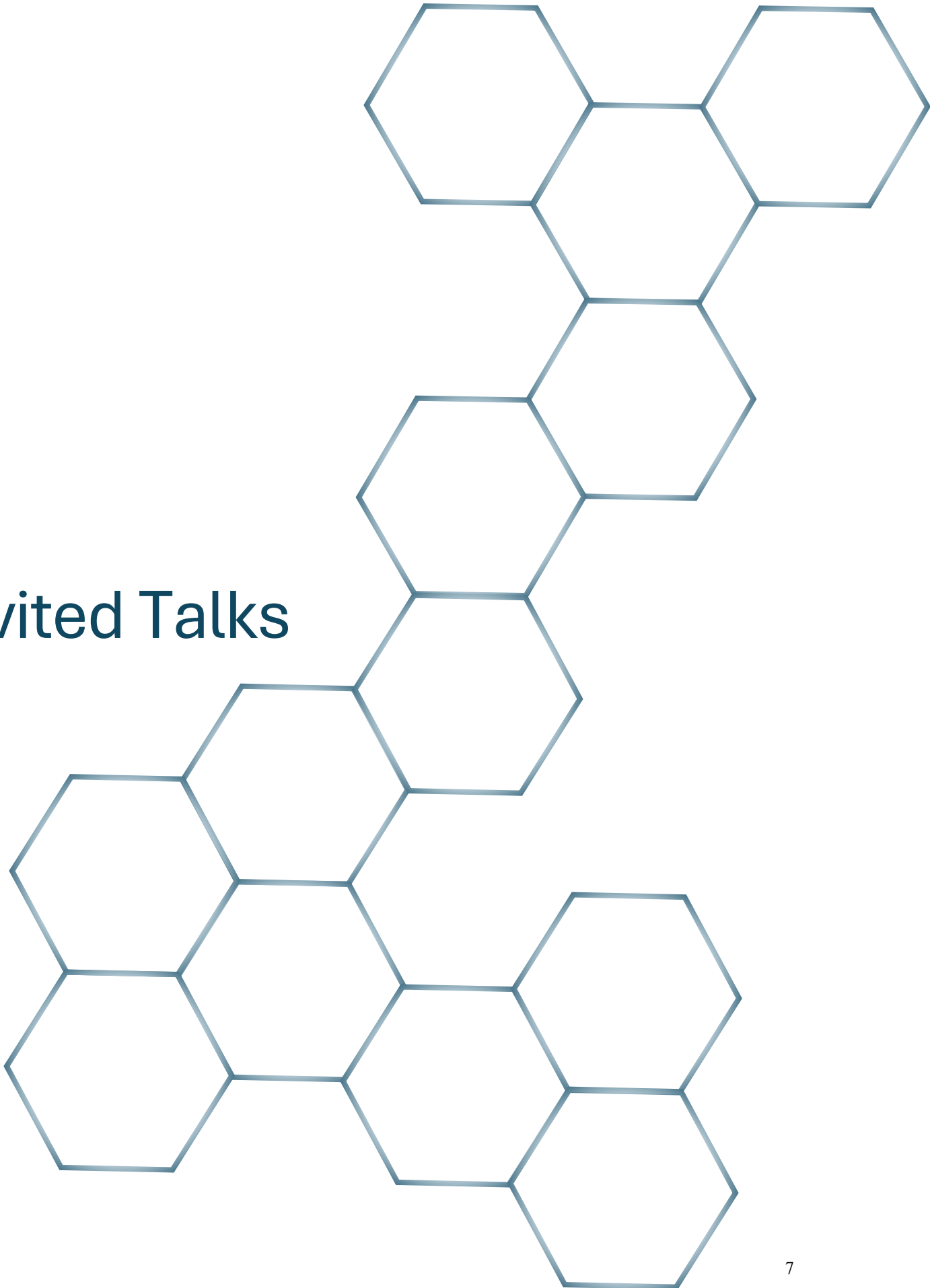
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Invited Talks



COLD H₂-Ar PLASMA INTERACTION WITH METAL HYDROXIDE AS A VERSATILE NANOFABRICATION TOOL OF METAL AND METAL@C_{gr} NANOPARTICLES: NICKEL AS A CASE STUDY

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Fabrication of tailored functional nanomaterials is at the heart of modern nanoscience and technologies. Among the numerous processing methods, common gas (H₂, CH₄, N₂, NH₃, O₂, Ar) assisted plasma interaction with given nano (in thickness) solid substrates has attracted more and more research interest. Plasma is a partially ionized gas, consisting of electrons, ions, molecules, free radicals, photons, and excited species, all of which are active species for the preparation and treatment of materials [1]. When high energy plasma species get into contact with a material, through gas-phase electron-impact or heavy-particle collisional ionization or dissociation of the feedstock gas, physical and chemical changes proceeded on the exposed surfaces [2]. Physical sputtering, chemical etching, reduction and oxidation, among others processes, may take place, leading to topographical and/or chemical transformations. Focusing on solid transformations, microwave plasma processing appeared as the most relevant. Surprisingly, it was seldom applied to metal hydroxides, despite their great reactivity due to their layered open structure. In this context, in the case of nickel system, interstratified α/β -Ni(OH)₂ [3] and turbostratic disordered α -Ni(OH)_{1-x}(CH₃CO₂)_x.nH₂O [4] derivatives were respectively prepared by co precipitation in water and in polyol. The recovered powders were compacted as pellets of 2 mm in thickness and then exposed to 90-10% H₂-Ar microwave plasma for different times. Interestingly, within these operating conditions starting, from one precursor or another, it was possible to produce ultrafine cubic Ni crystals (10-20 nm in diameter) coated or not by a thin graphite layer (2-3 nm in thickness) [5,6]. In one scenario, the hydroxide was directly reduced into the desired metallic phase, while in the second, it was simultaneously decomposed into metal oxide and metal carbide phases, which in turn evolved into metal@carbon core-shell nanoparticles.

[1] Z. Wang, Y. Zhang, Y. Cornelis Neyts, X. Cao, X. Zhang, B. W. L. Jang and C. Liu, ACS Catal., 8, 2093 (2018).

[2] F. Yu, M. Liu, C. Ma, L. Di, B. Dai, L. Zhang, Nanomaterials, 2019, 9, 1436S (2019).

[3] K. Lawson, S. P. Wallbridge, A. E. Catling, C. A. Kirk, S. E. Dann, J. Mater. Chem. A, 11, 789 (2023). [4] L. Poul, N. Jouini and F. Fiévet, Chem. Mater., 12, 3123 (2000).

[5] M-C. Dragassi, S. Haj-Khlifa, N. Menguy, M. Redolfi, S. Ammar, Int. J. Hydrogen Energy, 50, 1253 (2024).

[6] M-C Dragassi, S. Haj-Khlifa, N. Menguy, M. Redolfi, S. Ammar, Mater. Adv., 5, 5614 (2024).

IT-2

PLANT VIRUSES AS BIOTEMPLATES FOR MATERIALS AND THEIR USE IN NANOMEDICINE

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Plant viruses are increasingly being used in nanomedicine. Their capsids, composed of self-assembled protein subunits, are stable and have a uniform shape and size. Thanks to genetic or chemical modification of the capsid's proteins, various functional groups are exposed on their external surface, making it possible to use surface chemistry to graft molecules or nanoparticles. Many studies on plant viruses showed that nano-objects can not only be grafted on the virus capsid, but they can be also encapsulated within the virus cavity. Under certain conditions, these viruses can release their genetic material, leaving the protein capsid empty. Numerous objects (nanoparticles (NP), organic fluorophores, drugs, etc.) can then be encapsulated in the capsid, allowing the functionalization of the internal surface of the capsid.

In the first part of this work, I will present the synthesis and characterization of new nano-bio-hybrid materials which are soluble and stable in solution. Iron oxide nanoparticles were grafted onto the outer surface of three plant viruses. After purification, the resulting nano-biohybrids were characterized by different technics (DLS, TEM, XPS...). These nano-objects presented enhanced hyperthermal properties compared to those of free Np [1].

In the second part, we used plant viruses as drug delivery system. The size of the capsid allows a large number of therapeutic agents to be loaded into its cavity, thereby increasing concentration. The protein capsid improves drug solubility. The protection of these agents by this capsid also gives them a longer circulation time and greater cellular penetration. We demonstrated that antiviral molecules against poxvirus [2] can be encapsulated into the cavity of viruses in a high ratio, without affecting the virus's structural integrity. In addition we showed that in the presence of the encapsulated drugs the rate of infection decreased compared to the free drugs.

[1] Nguyen HA et al. *Nanomaterials* **2023**, 13(18), 2509

[2] Kappler-Gratias S et al. *ACS Infect. Dis.* **2021**, 7, 2370–2382

FROM NERVE REGENERATION TO OIL INDUSTRY: FUNDAMENTALS AND APPLICATION OF MAGNETIC NANOPARTICLES SYSTEMS

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Studies over the past few decades have demonstrated that superparamagnetic nanoparticles (NPs) are useful in biomedical fields such as cancer treatment, magnetic resonance imaging, drug delivery, and nerve regeneration. Magnetic hyperthermia (MH) involves raising the temperature of a system using magnetic NPs when exposed to an oscillating magnetic field, which facilitates the application of magnetic nanoparticles in nanotheranostics, for example. In addition, magnetic NPs can be utilized to improve nerve regeneration through magnetic-targeted cell therapy [1]. In industrial contexts, MH can decrease the viscosity of fluids used in Oil&Gas, pharmaceutical, chemical, and food industries [3,4]. The effectiveness of magnetic NP applications can be enhanced by adjusting their shape, size, composition, or degree of aggregation. Recent findings on magnetic NP applications along with studies on the anisotropy of cobalt ferrite (CFO) NPs for MH will be presented [5].

[1] P. A. Soto et al. *Acta Biomaterialia*, 2021, 130, 234-247.

[2] M. E. F. Brollo et al. *ACS Omega* 2023, 8, 36, 32520–32525S.

[3] M. E. F. Brollo. *ACS Appl. Nano Mater.* 2021, 4, 12, 13633–13642

[4] A. A. de Almeida et al. *ACS Appl. Mater. Interfaces* 2024

IT-4

X-Ray Magnetic Circular Dichroism: An Effective Technique for probing the electronic et magnetic properties of nanomaterials

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Due to their nanoscale dimensions and high surface-to-volume ratio, transition-metal nanoparticles exhibit essential magnetic properties such as superparamagnetism, spin canting, and magnetic anisotropy. These properties open the door to a wide range of applications, including biomedical imaging, medicine, magneto-optical devices, magnetic recording, and soil and water remediation. Additionally, magnetic properties can be optimized by refining synthesis methods or adjusting conditions within the same synthesis approach. For example, the "hard magnetic" nature of cobalt ferrite (CoFe_2O_4), combined with its exceptional physical and chemical stability, makes CoFe_2O_4 nanoparticles suitable for various technical applications¹. For data storage applications, $\text{Fe}_{3-d}\text{O}_4@\text{CoO}$ nanoparticles demonstrate enhanced magnetic anisotropy due to strong exchange-bias coupling between the ferrimagnetic $\text{Fe}_{3-d}\text{O}_4$ phase and the antiferromagnetic CoO phase^{2,3}.

Soft X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) at the L_{2,3} absorption edges are powerful techniques for probing the structure of nanoparticles. They provide insight into cation site symmetry, multiple valences, and other structural details. Thanks to chemical selectivity, these methods distinguish the contributions of each element to the magnetic properties of nanoparticles. Selective XMCD magnetization measurements add further detail about magnetic couplings within simple nanoparticles as well as in complex systems.

I present here the use of XAS and XMCD to analyze two types of magnetic nanoparticles. For $\text{Fe}_{3-d}\text{O}_4@\text{CoO}@\text{Fe}_{3-d}\text{O}_4$ nanoparticles, which are relevant for data storage applications, XAS and XMCD help determine the valence states, site occupancy of Fe and Co, and the nature of the core-shell interface⁵. In a second system, these techniques allow us to investigate the speciation of Co adsorbed on the surface of magnetite (Fe_3O_4), with implications for soil and water remediation applications⁶.

[1] N. Daffé, F. Choueikani, S. Neveu, M.-A. Arrio, A. Juhin, P. Ohresser, V. Dupuis, P. Saintavit, *JMMM* 460, 243-252 (2018)

[2] K. Sartori, G. Cotin, C. Bouillet, V. Halté, S. Bégin-Colin, F. Choueikani, B. P. Pichon, *Nanoscale* 11, 12946-12958 (2019)

[3] K. Sartori, D. Ihiwakrim, Ch. Lefèvre, S. Reguer, C. Mocuta, S. Bégin-Colin, F. Choueikani, B. P. Pichon, *Mater. Adv.*, 3, 8716 (2022)

[4] P. Ohresser, E. Otero, F. Choueikani, K. Chen, S. Stanescu, F. Deschamps, T. Moreno, F. Polack, B. Lagarde, J.-P. Daguette, F. Marteau, F. Scheurer, L. Joly, J.-P. Kappler, B. Muller, O. Bunau, Ph. Saintavit, *Review of Scientific Instruments*, 85, 1, 013106 (2014)

[5] K. Sartori, R. Lopez-Martin, F. Choueikani, A. Gloter, J.-M. Grenèche, S. Bégin-Colin, D. Taverna, J. De Toro, B. P. Pichon, *Nanoscale Adv.*, 6, 2903 (2024)

[6] L. Fablet, F. Choueikani, M. Pédrot, M. Kerdiles, M. Pasturel, R. Marsac, *Environ. Sci.: Nano* 10, 3051 (2023)

ELECTRON SPECTROSCOPIES FOR NANOMATERIALS ANALYSIS

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Electron spectroscopies are well-established techniques, largely employed for the investigations of the surface chemical composition of a huge number of solid-state materials. The peculiarity of these techniques lies in their ability to probe a very tiny layer of the investigated materials, within the range of $1 \div 10$ nm. Therefore, they represent a powerful tool for the study of nanomaterials. As it is well known, within the big family of nanomaterials are included nanoparticles, nanorods, nanowires, nanofilms, 2D-materials, etc., basically, all materials characterized by at least one dimension in the range of nanometers scale. The most popular techniques employed to study the nanomaterials are the microscopies, like SEM, AFM, STM, etc., but also spectroscopies like Raman spectroscopy, FTIR, Energy dispersive analysis (EDS), etc. However, the most surface sensitive techniques are the electron spectroscopies, which can provide information on the chemical state of the detected elements. They include X-ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES), Ultraviolet Photoelectron Spectroscopy (UPS) and Energy Electron Loss Spectroscopy.

This presentation will give an overview of the main results obtained from the study of various nanostructured materials. Depending on the materials, it was alternatively employed XPS, AES and UPS, in order to determine the surface elemental composition of nanoparticles, nanofilms and 2d-materials [1], surface elemental distribution performed by XPS and AES microscopies [2], the work function calculation by UPS [3] and the D parameter used for the detection of the concentration of C-sp² and C-sp³ hybridization in carbon-based materials, but also to detect the chemical modifications passing from graphite, to graphene oxide and reduced graphene oxide [4].

[1] E. Bolli, S. Kaciulis, A. Mezzi, *Coatings* 10, 1182 (2020).

[2] A. Mezzi, S. Kaciulis, M. Brucale, D. Gentili, M. Barbalinardo, M. Durso, M. Melucci, M. Cavallini. *SIA* 48, 626 (2016)

[3] A. Mezzi, E. Bolli, S. Kaciulis, A. Bellucci, B. Paci, A. Generosi, M. Mastellone, V. Serpente, D.M. Trucchi. *Nanomaterials* 13, 1430 (2023).

[4] S. Kaciulis, A. Mezzi, P. Soltani, T. de Caro, H. Xia, Y.L. Wang, T. Zhai, M. Lavorgna. *SIA* 50, 1089 (2018).

Thermodiffusion in a multicomponent lyotropic mixture in the vicinity of the critical micellar concentration by using the Z-scan technique

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Thermodiffusion in a lyotropic mixture of water and potassium laurate is investigated by means of an optical technique Z-scan distinguishing the index variations due to the temperature gradient and the mass gradients. A phenomenological framework allowing for coupled diffusion is developed in order to analyze thermodiffusion in multicomponent systems. An observable parameter relating to the mass gradients is found to exhibit a sharp change around the critical micellar concentration, and thus may be used to detect it. The change in the slope is due to the markedly different values of the Soret coefficients of the surfactant and the micelles. The difference in the Soret coefficients is due to the fact that the micellization process reduces the energy of interaction of the ball of amphiphilic molecules with the solvent. We have found that the response of the mixture of amphiphilic molecules and water is sensitive to the aggregation state of that mixture. The jump in just above the CMC is due to the nondiagonal diffusivity $D_{m,KL}$ (m represents micelles and KL is the amphiphile potassium laurate) expressing the sensitivity of micelle diffusion to the gradient in the mass fraction of free KL . Although the Soret ratios have opposite signs, the thermophoreses of both species occur toward warmer temperatures. The sharp difference in the Soret ratios endows with the capacity of evidencing the micelle formation in the lyotropic mixture and determining the CMC.

CARBON-BASED PARTICLES AS NEW TOOLS TO INHIBIT AN AGENT RESPONSIBLE FOR A MAJOR SEXUALLY TRANSMITTED INFECTION

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Sexually transmitted infections (STIs) are a major public health problem. More than one million sexually transmitted infections are acquired every day worldwide, the majority of which are asymptomatic. Every year, 374 million people contract one STI. *Chlamydia trachomatis* is a bacterium that causes one of these STIs.

To tentatively limit the growth of this pathogen, we designed solid antibiotics through a hydrothermal process transforming ciprofloxacin (Cip) into Cip carbon-based particles (CNP-Cip), never evaluated against this bacterium yet. The aim of this chemical transformation is to take advantage from CNPs colloidal feature, improving solubility and transport across biological barriers, while maintaining the antibacterial activity of the starting drug.

We therefore characterized the resulting particles and assessed, for the first time, their activity against *C. trachomatis*. We observed that some of these objects display a higher antibacterial activity than the parent Cip, while targeting the same bacterial protein. This result is essential in the field of nanobiotechnology, since it establishes that CNPs-Cip produce a better therapeutic effect.[1]

[1] Ciprofloxacin carbon-based particles to inhibit *Chlamydia trachomatis* growth. Submitted to *Nanomedicine: Nanotechnology, Biology, and Medicine* (manuscript number: JN2024778).

From Carbon Dots to Nanographenes: Photophysics and Photonics of Optical Carbon Nanomaterials

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The discovery of carbon nanodots and nanographenes has recently triggered a strong research interest in view of their fascinating optical properties, which break the paradigm of Carbon as a “black” material and pave the way to a variety of applications in optoelectronics, photocatalysis, nanosensing, photonics and bioimaging. Carbon dots can be synthesized through several straightforward chemical routes and display a favourable combination of tunable optical responses, low toxicity, strong absorption and emission transitions, high emission quantum yields. On the other hand, the controlled deformation and engineering of the sp^2 carbon network in nanographenes, opens unparalleled opportunities for the modulation of optical and electronic properties with ultimate atomic precision.

This contribution is focused on some of our latest work on the fundamental photophysics and photonic applications of these two optical carbon nanomaterials. In particular, I will discuss our recent efforts to use carbon dots as active materials to build a family of laser and random laser light sources which can be tuned throughout the visible spectral range, and our recent demonstration of functional light-emitting microcomposites obtained by coupling nanographenes to polystyrene microbeads, with applications in anticounterfeiting, metrology and information encoding. The results demonstrate the high potential and extreme versatility of carbon-based nanomaterials for prospective applications in “soft” photonics.

Carbonaceous Nanomaterials for Agrotechnological and Environmental Applications

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Due to their multifunctional properties, low toxicity, biocompatibility, and biodegradability, carbon-based nanomaterials have found extensive use in agrotechnological and environmental applications. Additionally, these nanomaterials can be synthesized through green methods using renewable raw materials, further enhancing their sustainability and eco-friendliness. Graphitic carbon nitride (g-C₃N₄), a metal-free visible-light photocatalyst, has shown great potential for environmental decontamination. Integrating magnetic nanoparticles (Fe₃O₄) with g-C₃N₄ enhances its optical, textural, and reactive properties, creating magneto-responsive adsorbent platforms that are easily recoverable and reusable. This study developed magnetic nanocomposites using Fe₃O₄ nanoparticles with nanoflower morphology that offers a cost-effective and eco-friendly solution for treating dye-contaminated water without pH adjustments, making it highly relevant for the dyeing industry. Carbon dots (CDs) are nanoscale carbon-based materials that gain significant attention in agriculture due to their unique properties, such as biocompatibility, low toxicity, and excellent fluorescence. These nanomaterials are used to enhance crop productivity through improved nutrient delivery, plant growth promotion, and stress resistance. Furthermore, they have shown potential in protecting crops by acting as carriers for pesticides or antimicrobial agents, reducing environmental contamination. Their eco-friendly nature makes them a promising tool for sustainable agricultural practices. This study proposes the engineering of carbon nanoparticles for use as nanofertilizers. Carbon dots are synthesized from different raw material sources, and core and surface modifications are studied based on synthesis parameters. The materials are tested in plant greenhouses and field trials, aiming at their translation to commercialization.

CHEMICAL SENSOR ARRAYS WITH FLUORESCENT CARBON QUANTUM DOTS

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Water and soil pollution has become a pressing issue due to intensive human activities. Addressing this challenge requires diverse strategies, such as the rational use of agrochemicals, advanced oxidative processes, adsorptive materials for waste treatment, and pollutant monitoring. Notably, conventional analytical tools like HPLC or MS are unsuitable for *in situ* monitoring. In contrast, chemical sensors offer significant advantages, including portability, rapid response, and real-time detection of chemical species. Among modern sensor technologies, fluorescent chemical sensor arrays, though less explored, show great promise. In this study, we present a “turn-off-on” sensing mechanism utilizing fluorescent carbon quantum dots (C-dots) and nanometric quenchers to quantitatively detect glyphosate (GLY) in water and differentiate it from common interferents such as aminomethyl phosphonic acid (AMPA) and glycine (GLYC). While GLY, AMPA, and GLYC quench the fluorescence of C-dots at similar rates, hampering discrimination, we addressed this limitation by integrating three nanometric quenchers—Ag nanoparticles, 2H-MoS₂, and graphene oxide—into the sensor design. These quenchers suppress the initial fluorescence of the C-dots, which is subsequently recovered upon the introduction of pollutants. Crucially, the fluorescence recovery patterns are unique for each pollutant, enabling the sensor array to distinguish GLY even in the presence of AMPA and GLYC. Using principal component analysis (PCA) for dimensionality reduction, the sensor array achieved accurate quantification of GLY over a wide linear range (1.18 μM to 5.18 μM , $R^2 > 0.99$) with a detection limit of 0.35 μM (S/N = 3), well below the regulatory limits set by Brazilian, US, and European standards. This study demonstrates the potential of tailored quenchers to modulate pollutant interactions with C-dots, advancing the development of effective and selective chemical sensor arrays.

Directional Molecular Self-Assembly for Photonics and Spintronics

F. Silly

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Engineering novel organic materials through molecular self-assembly has received tremendous attention during the recent years.

A pragmatic approach consists in using blocks that can form distinct architectures through selective and directional multiple bonds. Molecular self-assembly through hydrogen bonds has been widely investigated during the last years, but there are in comparison few reports on organic structures resulting from alternative selective and directional intermolecular interactions as halogen bonds.

We present a successful strategy to obtain a self-assembled material stabilized by halogen bonding with enhanced mechanochromic aggregation-induced emission. The metabromophenyl-substituted tetraphenylethene fluorophore exhibits an emission which is more red-shifted compared to the phenyl-ring-substituted tetraphenylethene fluorophore in film. The Br-molecule molecules self-assemble into uniform ball-like aggregates with high photoluminescence quantum yield, which indicates that the molecular conformation and intermolecular interactions are different from those in the crystalline state.

We also investigate the structural and magnetic properties of halogen-bonded films of two β -diketonato complexes sharing the same skeleton but one functionalized with peripheral bromine atoms and the other with iodine atoms. Experimental measurements reveal that the Cu-complexes preferentially lay flat on the graphite surface, but the two molecules self-assemble into distinct arrangements. The magnetic hysteresis loops show that the organic thin film remains paramagnetic at 2 K but the magnetic signal is stronger with the iodine-molecule, highlighting the impact of molecular arrangement on magnetic properties.

Decomposition of H₂O₂ by iron oxide and sulfide nanoparticles

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The hydrogen peroxide H₂O₂ exhibits a number of families of reactions that are important for energy, biology, the environment, industrial chemistry (including bleaching, organic synthesis, polymers, and medicine), or both. This versatility results from the fact that H₂O₂ exhibits both oxidizing and reducing properties because of the oxygen's (O⁻¹) oxidation state. Particularly, the chemical reactions and interactions between H₂O₂ and iron-based minerals, namely ferrites and pyrite, proved to be important in a variety of contexts, like the environment and energy, and including those pertaining to astronomy/astrobiology or even the origin of life. In the reaction between hydrogen peroxide and minerals, the creation of extremely reactive free radicals is primarily the crucial point. This interaction is intensified at the nanoscale and, at the same time, it is strongly related to the morphology, composition, and electronic and chemical properties of the nanoparticulated system. This presentation will discuss three lines of study on the aforementioned topic. Firstly, the impact of the composition and structure of the whole of core-shell iron oxide (FeO-Fe₃O₄) nanoparticles on the surface reaction with H₂O₂ is demonstrated. Secondly, studies on the impact of morphology, nucleation, and growth of pyrite nanoparticles due to the presence of Na in the synthesis in the chemical activity for the decomposition of H₂O₂ will be presented. The results presented above concerning the catalytic activity are obtained by EPR spectroscopy with a spin trap. Then, an indirect way, as is usual, to study the formation of free radicals by any spectroscopic technique. In this way, as a final part of the presentation, theoretical and experimental results from FTIR spectroscopy for in-situ reactions are being developed, aiming to explore the possibility of using this technique in order to obtain a direct measurement of the H₂O₂ decomposition and the chemical species formed by it.

FABRICATION OF COMPLEX THREE-DIMENSIONAL MICRO- AND NANODEVICES FOR PHOTONICS AND MICROFLUIDICS

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In this talk, I will describe the research potential of a laboratory for additive microfabrication based on two-photon absorption photopolymerization (TPA), which is currently being implemented at IF-USP. TPA is a ultrashort laser-based fabrication technique that leverages the nonlinear nature of the two-photon absorption process to fabricate 3D microstructures with arbitrary geometries and resolutions down to hundreds of nanometers [1]. TPA stands out for its versatility and simplicity, eliminating the need for multiple processing steps, lithographic masks, and highly corrosive agents. Furthermore, a wide range of materials can be used as photoresists, or incorporated into them, allowing customization of the physical, chemical, or biological properties of the fabricated microstructures to enable various applications. Another significant advantage of TPA is the ability to fabricate microdevices onto different substrates, paving the way for the direct integration between photonic chips, optical fibers, and microfluidic systems. This enables leveraging photonic technologies to develop *in situ* analysis tools for microfluidic systems. One of my projects in this direction focuses on integrating microfluidic systems with an on-chip mid-infrared spectroscopy photonic system [2] to enable an *in situ* strategy for biochemical detection and quantification with high acquisition rates and sensitivity. Additionally, I aim to explore the combination of photonic and microfluidic technologies to develop a method for determining the size of nanoparticles and separating these particles by size. This will be highly relevant for studying the role of high-density lipoproteins (HDLs), which have dimensions on the order of tens of nanometers, in cardiovascular diseases [3-4].

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HARD-AXIS COLLAPSE AND RECOIL CURVES LYING OUTSIDE THE MAJOR HYSTERESIS LOOP IN FERROMAGNETS

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Magnetic hysteresis is, virtually, the most prominent and intriguing phenomenon of ferromagnetism. It has been recently discovered that systems which display magnetization hard-axis collapse (HAC), i.e., sharp peaks in the angular variations of the remanent magnetization and coercivity centered 90° off of the easy-magnetization direction, also show recoil branches that lie way outside the major hysteresis loop [1]. This phenomenon, referred to as a recoil-curve overshoot (RCO), together with enhanced remanence and coercivity values, results in an important increase of the hysteresis loop's area. Systems presenting RCO also feature hysteresis branch crossings just before saturation, hysteretic instead of reversible magnetization processes in the region between the saturation and remanence states, and also a great temperature stability of both HAC and RCO.

Here we present a review on the key features of HAC and RCO together with the responsible for their disclosure magnetization reversal. Our recent results [2-5] strongly support the hypothesis that both phenomena arise from exchange coupling within grains which magnetizations split into pairs of exchange-coupled monodomains with a local easy-axis misalignment. The latest findings on these intriguing phenomena, which should be rather general features of polycrystalline magnetic systems' hysteresis and observed in a variety of systems, indicate that further theoretical and experimental investigations may come out with important new applications.

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EFFICIENT AND STABLE PEROVSKITE SOLAR CELLS: NEW MATERIALS AND MODELING

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Perovskite solar cells (PSCs) have attracted widespread attention in academia and industry due to their high-power conversion efficiency (PCE) and potential for low-cost, sustainable, and large-scale manufacturing. We have incorporated two-dimensional (2D) materials to enhance the performance of double-cation mixed halide perovskite ($\text{Cs}_{0.17}\text{FA}_{0.83}\text{Pb}(\text{I}_{0.83}\text{Br}_{0.17})_3$) solar cells. We developed a Nb_2O_5 ETL layers adding $\text{Ti}_3\text{C}_2\text{T}_x$ MXene into a solution processable ink [1]. The addition of MXene increased the PCE (19.46% for the champion device) and the stability (96% of its original PCE after 500 hours) compared to pristine devices. The improved performance of the Nb_2O_5 - Ti_3C_2 is attributed to the alignment of the energy bands between perovskite and the ETL layer. In inverted or p-i-n PSCs we used an ultra-thin poly(methyl methacrylate) (PMMA) layer to passivate interfacial defects between the perovskite and the ETL layer [2]. With the addition of $\text{Ti}_3\text{C}_2\text{T}_x$ MXene resulted in improvement of the PSC photovoltaic parameters, boosting their efficiency to $21.30 \pm 0.51\%$ (22.1% for the benchmark PSC). The enhanced performance is attributed to a reduction of trap state densities accompanied by mitigation of non-radiative recombination. The PMMA:MX based devices maintained 95% of their original PCE after 3000 h (ISOS-D-11) and took 3X longer to reach T80 compared to the control PSC under heat and light soaking (ISOS-L-2). In another study [3], the deposition of Nb_2O_5 as an electron transport layer via slot die coating was systematically investigated. These Nb_2O_5 layers were used as electron transport layers in n-i-p perovskite devices. Under optimal coating conditions, efficiencies up to 12 % were obtained. A conceptual framework for characterizing photovoltaic devices by integrating cyclic voltammetry (CV) and impedance spectroscopy (IS) will also be presented [4]. We derive comprehensive analytical expressions for current-voltage relationships and complex admittance.

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IT-16

Advances in Flexible Organic and Perovskite Photovoltaics for Sustainable Energy Generation

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The development of solar energy technologies has driven the search for more efficient and versatile solutions. In this context, flexible photovoltaics have emerged as a promising approach for sustainable energy generation. Flexible organic photovoltaics rely on organic semiconductor materials, which offer notable benefits such as low production cost, reduced weight, and the ability to be manufactured on flexible substrates. These characteristics make them ideal for applications in portable devices, smart clothing, and even integrated buildings. Continuous advances in organic materials and manufacturing techniques have led to significant improvements in their conversion efficiency, stability, and durability [1-2]. On the other hand, perovskites have gained considerable attention due to their exceptional light absorption and charge transport properties. Flexible perovskite photovoltaics have demonstrated very high conversion efficiencies, with the potential to surpass other solar cell technologies. Additionally, they can be manufactured using thin-film deposition techniques, enabling the creation of flexible and semi-transparent solar cells. However, both types of flexible photovoltaics face specific challenges. Stability and durability remain concerns for organic photovoltaics, while perovskites suffer from degradation when exposed to moisture and light. Research is ongoing to overcome these challenges and enhance the efficiency and lifespan of these devices

Development of nanostructured core/shell systems for controlled drug release

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Drug Delivery Systems (DDS) can be designed to target specific tissues, with release mechanisms controlled by physicochemical triggers such as pH, temperature, or light irradiation. These features help minimize unwanted side effects. To enhance the efficiency of DDS platforms, it is widely recognized that innovative synthesis routes are essential for achieving precise control over parameters like size, shape, porosity, and surface functionalization. In this study, we first present the synthesis of mesoporous silica-coated magnetite nanoparticles (MNP@mSiO₂) capped with polyelectrolytes (PE). The morphology and physical properties of the system's components were thoroughly characterized. Drug release studies showed that uncapped mesoporous silica nanoparticles loaded with TCH released over 90% of the drug within 48 hours, whereas the PE-capped nanoparticles released only 30%, due to the PE layer hindering drug diffusion. In the second part of the study, the PE capping was replaced with silane functionalization (APTES hydrolysis) to develop a pH-triggered release system. The functionalized nanoparticles released approximately 20% of DOX at pH 6.6 or 7.4 but showed a significant release of up to 80% at pH 5.5. Lastly, preliminary results are presented on the microfluidic synthesis of magnetite nanoparticles, and a multistep microfluidic approach that could be used for synthesizing mesoporous silica-coated magnetite nanoparticles (MNP@mSiO₂).

FROM NANOPARTICLES TO 4D-PRINTED DEVICES: ADVANCEMENTS IN DRUG DELIVERY PLATFORMS

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Nanostructures have emerged as promising platforms for controlled drug delivery, offering precise release and targeting capabilities that enhance therapeutic efficacy while minimizing side effects. [1] Additionally, the diverse physicochemical properties of these nanoscale structures enable controlled release through various external stimuli. In this context, magnetic nanoparticles, which generate heat under an oscillating magnetic field, are being explored as an innovative platform for intelligent drug release devices.

We present two novel materials that utilize iron oxide (Fe_3O_4) nanoparticles as active agents for the controlled and contactless delivery of non-steroidal anti-inflammatory drugs (NSAIDs). The first system consists of complex core-shell architectures, with Fe_3O_4 cores encapsulated in a mesoporous SiO_2 shell, demonstrating high loading capacity and controlled release of specific NSAIDs via external magnetic fields. [2] The second example combines Fe_3O_4 nanoparticles with different polymers to create commonly 3D-printable magnetically activated heat generators. [3] In addition, this polymer-based composite enables the incorporation of specific NSAIDs, with the additional capability of being 3D-printed into customized shapes. As a 4D-printed drug delivery device, it achieves enhanced control over drug release through magnetic field application, offering improved regulation compared to passive release mechanisms.

These results highlight the potential of magnetic nanoparticle-based systems for the development of intelligent, controlled drug delivery platforms. Both approaches effectively leverage external magnetic fields to regulate drug release, offering promising opportunities for personalized therapeutic applications.

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Magnetic Anisotropy and Exchange Bias in Size-distributed Ultrasmall Nanoparticle Systems

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Understanding the thermal dependence of the magnetic properties of nanomaterials is mandatory to enable and develop new applications. There are many parameters that influence such properties and their originated effects. For instance, saturation magnetization m_s and magnetic anisotropy energy K become size-dependent at the nanoscale. Consequently, thermal variations impose effects on magnetic materials, such as superparamagnetism. We investigated the influence of polydispersity on the thermal dependencies of coercivity $H_c(T)$ [1] and bias field $H_{exc}(T)$ [2] of ultrasmall core@shell magnetic nanoparticles in compressed powder and ferrofluids. The analysis of the thermal behaviour of these two quantities allows us to shed light on the physical processes involved. By considering the necessary conditions for magnetic coupling and the volume-dependent transition to the superparamagnetic state, we demonstrate that the thermal dependence of exchange bias is due to two different temperature-modulated effects. The first effect is the freezing of interfacial spins and the second is the changing populations of superparamagnetic and blocked nanoparticles. Our results demonstrate that even at very low temperatures, the fraction of nanoparticles subjected to superparamagnetic relaxation has an important effect on the magnetic behaviour of nanoparticle systems, being also responsible for the modulation of coupling and, thus, the exchange bias effect.

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MAGNETIC COLLOIDS IN EMIM TFSI, PROPYLENE CARBONATE AND THEIR MIXTURES FOR IMPROVED THERMOELECTRIC PERFORMANCE

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Liquid thermocells hold potential for converting low-grade waste heat into electricity [1]. This study explores the potential to enhance thermoelectric conversion in these cells by designing innovative ionic liquid-based colloids containing charged magnetic nanoparticles (NPs) with optimized properties [2]. Core@shell NPs (CoFe₂O₄@g-Fe₂O₃) of various sizes with three different coatings were tested in EMIM TFSI, an ionic liquid with high electrical conductivity. PAC₆MIM⁺Br⁻ (1-(6-hexylphosphonate) 3-methyl imidazolium bromide) emerged as the most effective ligand due to its phosphonic group, leading to nanoparticle clusters in water and a few NPs in EMIM TFSI. To optimize viscosity and electrical conductivity, dispersions in binary mixtures of propylene carbonate (PC) and EMIM TFSI were investigated, focusing on the sample with NPs of ~ 7 nm diameter. A pumping and heating procedure yielded stable dispersions, reducing nanoparticle cluster size to 1-2 NPs in EMIM TFSI and a few in PC and their mixtures. The mixture with an IL mole fraction of ~0.2–0.3 showed maximum electrical conductivity, presenting a promising candidate for further thermoelectric studies [3].

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Design of core/shell multifunctional nanoparticles for environmental remediation

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Magnetic nanoparticles (MNPs) are used in a wide range of applications and hold great promise for providing solutions for actual challenges in environmental remediation, energy, and medicine. What distinguishes this family of materials is the remarkable versatility to tune their properties by adjusting factors such as size, shape, composition, crystallinity, and interactions. Furthermore, materials with different functionalities can be combined in a single nanoparticle, allowing the design of multifunctional materials. In this context we present the strategies followed to develop magnetic nanocatalyzers for environmental remediation. Our approach involves designing MNPs with core/shell architecture, optimizing the shell properties to catalyze the decomposition of organic contaminants while adjusting the magnetic response of the core to induce local heating in presence of ac magnetic field, i.e. magnetic hyperthermia, thus enhancing the kinetic reaction by the temperature. The optimization of the magnetic properties also enables the magnetic harvesting and reuse of the nanocatalysts in successive cycles enhancing its efficiency.

The catalytic performance was optimizing by tuning the shell composition to enhance the production of reactive oxygen species (ROS), via Fenton-like reactions. These species, especially the $\bullet\text{OH}$ and $\bullet\text{OOH}$ free radicals, are highly effective in degrading organic pollutants. With this aim copper-doped iron oxide MNPs were fabricated and their ROS production and ability to degrade organic compounds was analyzed. We found that while Fe^{2+} is the most active ion at room temperature, it rapidly oxidizes to Fe^{3+} , diminishing its efficacy. In contrast, copper exhibits lower activity than Fe^{2+} at room temperature but demonstrates improved performance at higher temperatures.

Furthermore, the magnetic anisotropy of the MNPs core can be precisely controlled to induce magnetic hyperthermia. This effect increases the reaction kinetics through temperature elevation, enhancing the catalytic performance. The synergistic combination of magnetic and catalytic properties improves the overall kinetics and efficacy, making these nanostructures highly promising for treating high-temperature industrial wastewater and offering compelling solutions for environmental remediation.

Magnetic field-driven structural and magnetic behaviour of Ferrofluids based on High-Moment Nanoparticles

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In the recent years, ferrofluids (FFs) based on magnetic nanoparticles coated with an organic surfactant are extensively used in a broad range of applications [1]. Understanding the mechanism of cluster formation, driven by an external magnetic field, and the factors that contribute to complete cluster dissociation, is pivotal for better ferrofluid’s magnetic manipulation for various applications. In this work, we focus on high-moment magnetic particles because of their fast response to magnetic fields of moderate strength. A complete model of the FF including the structural and magnetic particle parameters characteristics, the inter-particle interactions as well as the interaction with the fluid is developed and applied in two representative cases of high-moment materials-based FFs, which are experimentally synthesized: 1) the CoFe₂O₄ multicore particles-based FFs of 60nm size [2] and 2) the FeCo alloy ones of 10nm size [3]. The Diffusion Limited Cluster Aggregation method [4] is employed to study the time evolution of the FFs and the optimum conditions for the formation of field-driven structures at room temperature. Importantly, the conditions for fast cluster dissociation after removing the field are studied for the first time, suggesting a completely reversible process, which results to the initial FF structure; in this way the FF can be ‘reused’.

The numerical simulations demonstrate that: a) the high magnetic moment plays significant role in the cluster aggregation rate in the presence of the field and b) the steric interactions due to the presence of the surfactant coating result to the completely reversibility of the cluster dissociation process.

This study opens new perspectives for controlling remotely the magnetic properties and the morphology of field-driven structures for novel FF-based green applications.

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Oral Communications



IN SITU OPTICAL PROBING ON THE CAROTENOID DEGRADATION KINETICS DURING *IN VITRO* OXIDATION OF HIGH-DENSITY LIPOPROTEINS

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High-density lipoproteins (HDL) have been comprehensively investigated in light of their atheroprotective ability [1]. In this context, HDL quality is typically evaluated considering its cholesterol efflux and antioxidant capabilities, both strongly dependent on particle composition, morphology, and number [2,3]. These functionalities are usually attributed to the apolipoprotein AI (Apo-AI), however, carotenoids may occasionally show the potential to reduce the risk of cardiovascular disease (CVD). Recently, McEneny et. al [4] investigated lycopene-rich diets, which showed an increase in paraoxonase1 (PON1) activity as lycopene binds to ApoA-1 reducing lipid peroxidation and reduced serum amyloid A (SAA). However, Carroll et al. [5] observed no reduction or delay in low-density lipoproteins (LDL) oxidation via supplementation with beta-carotene or lycopene. Further, Solakivi et al. [6] observed that HDL can enhance LDL susceptibility to oxidation depending on polyunsaturated fatty acid content. Therefore, the carotenoid antioxidative mechanism and efficiency within lipoproteins remain elusive. In this context, here we investigated the chemical and structural modifications induced by *in vitro* oxidation of native HDL collected from two normolipidemic disease-free donors, which differ greatly in carotenoid content. Small angle X-ray scattering (SAXS) and dynamic light scattering (DLS) probed structure, size, and interparticle interactions as a function of oxidation time. In spite the carotenoid difference between individuals, the experimental results show very similar native HDL particle structure and size. Regarding the oxidative stress, agglomeration was observed in very long-lasting oxidation periods. Still, it is unlikely this type of aggregation actually occurs under *in vivo* conditions. UV-Vis spectrophotometry, non-linear optics (Z-Scan) and high-performance liquid chromatography (HPLC) inspected the temporal evolution of carotenoid and lipid degradation. The UV-vis absorbance and Z-Scan thermo-optical effect initially reduce with oxidation, elucidating the kinetics of carotenoid interaction with free radicals. The difference in carotenoid content has no apparent influence on the prevention of lipid oxidation. Notwithstanding, other factors such as the deterioration of the proteome cannot be ruled out. In conclusion, this work provides insights into the protective role of carotenoids in the oxidative stress of HDL, shedding light on the extent of their capability to prevent structural and compositional alterations that impair functionality. This work was supported by Conselho Nac. de Des. Cient. Tecnológico (CNPq) in the context of the INCT-FCx (Project nº 465259/2014-6).

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Multi-Scale and Hierarchical Cluster Organization in Nitrogen-Enriched Carbon Dots Dispersions

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Carbon nanodots are carbon-based nanomaterials with exceptional photoluminescent properties. These easily synthesized nanostructured materials are also of great interest due to their appealing biophysical-chemical characteristics, such as biocompatibility, high sensitivity to metal ions in solution, photocatalytic properties, and low toxicity [1]. In this study, we investigate nitrogen-enriched carbon nanodots (N-CDs) synthesized by thermally induced decomposition [2]. Their size, structure, and morphology in powder form were investigated in two conditions: pristine (as produced by the synthesis) and freeze-dried, by combined analysis of TEM and XRD. Nanodots aqueous dispersions at different pH conditions (2, 7, and 12) were studied by synchrotron SAXS experiments. In pristine form, different amounts of precipitate could be observed at the macroscopical scale, while for the freeze-dried powder little to no precipitate was formed, especially in pH 12. Time-dependent measurements were performed to investigate the sedimentation processes with the pristine N-CDs. The structure of the dispersed N-CDs is highly dependent on the C/N ratio used in the synthesis procedure, which can be surface and mass fractals. Also, the presence of large agglomerates was detected by DLS experiments. Ultimately, the colloidal stability was studied with zeta potential measurements, which revealed an increase of the negative surface charge as the medium becomes more alkaline, in agreement with the deprotonation of carboxyl surface groups [3]. Overall, the whole of the results shed light on the nanoscale ordering of N-CD dispersions as a function of pH allowing a deeper understanding of the colloidal stability of the system.

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A DETAILED MAGNETIC ANALYSIS OF THE TRANSITION BETWEEN WEAKLY AND STRONGLY INTERACTING SYSTEMS OF FERRITE NANOPARTICLES

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By altering the concentration regimes of ferrite-based nanoparticle samples, this work shows the changes in magnetic properties through the analysis of results obtained from magnetization techniques such as remanence, hysteresis, first-order reversal curves, AC susceptibility, and low-field magnetization. The samples are spinel-type nanocrystals consisting of a ferrite core coated with a maghemite shell, synthesized as aqueous colloidal dispersions via a core-shell strategy. These nanoparticles exhibit high anisotropy, attributed to enhanced surface contributions. Moreover, the blocking temperature shifts to higher values as the interparticle distance decreases. The samples investigated include both diluted and concentrated ferrofluids, as well as powders with different degrees of compaction. They display a frequency-dependent blocking temperature, which is well explained by the Vogel-Fulcher law, incorporating a phenomenological temperature associated with the magnitude of dipolar interactions between particles. The fractional change in peak temperature per frequency decade reveals particle interactions in diluted liquids and indicates a spin-glass-like state in powder samples. FORC diagrams corroborate the increase of demagnetizing forces, attributed to dipolar interactions, as the concentration of interacting nanoparticles increases. Finally, comparing three remanent magnetization techniques reveals similar results, underscoring the presence and enhancement of exchange interactions in more compacted regimes—systems with shorter interparticle distances—thus promoting an additive magnetizing effect.

OC-4

Effect of pressure of sputtering chamber in gas sensing and photocurrent properties of ZnO thin films

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Nanostructured oxide materials are currently used as biosensors in technological applications. These materials are of great interest due to their potential for use in medical diagnostics, as they enable rapid, non-invasive, and low-cost evaluations. In this work, zinc oxide (ZnO) films were produced by the sputtering deposition method, varying the working pressure, in order to obtain materials with specific features which can be used as gas sensors. Surface analysis using SEM revealed the formation of microrods and two sizes of grains, one larger than 1 micrometer and the other smaller than 500 nm. X-ray diffraction analysis revealed the formation of ZnO's wurtzite phase with preferential orientation along the [002] direction. It was determined that the film thickness decreases as the working pressure is increased. XRD data analysis also indicates that the mean crystallite size and lattices constants decreases as the working pressure is increased. UV-Vis spectroscopy results revealed that the band gap energy of the films does not show a clear tendency with the working pressure. However, Urbach Energy increases from 0.1 to 0.3 eV, suggesting the formation of more defects as the film thickness become thinner. The temperature dependence of the resistivity of the films in the range from 300 to 573K shows a typical semiconducting behavior and indicates the presence of two activation energies. Photocurrent measurements for the films showed a good sensitivity to UV light. Data analysis indicates the presence of trap energies at 0.58 and 0.63 eV, suggesting fast and slow response, respectively. Tests of sensor response using methane gas were carried out, which showed that the ZnO films can be used as a gas sensor material. [1] Amiri, V.; Roshan, H.; Mirzaei, A.; Neri, G.; Ayesh, A.I. Nanostructured Metal Oxide-Based Acetone Gas Sensors: A Review. *Sensors* 2020 [2] Q. A. Drmosh, I. Olanrewaju Alade, M. Qamar, S. Akbar, *Chem. Asian J.* 2021 [3] Kumar, Nishant & Srivastava, Anchal. Faster photoresponse, enhanced photosensitivity and photoluminescence in nanocrystalline ZnO films suitably doped by Cd. *Journal of Alloys and Compounds.* (2017).

Tailoring magnetic anisotropy and hyperthermia efficiency in γ -Fe₂O₃/CoFe₂O₄ core/shell nanoparticles through shell thickness control

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Magnetic Nanoparticles (MNPs) with a core/shell structure are of great interest due to their unique properties, which can be used in many fields of application, e.g., in magnetic hyperthermia for cancer treatment [1]. Magnetic hyperthermia involves injecting MNPs into the body and then exposing them to a high-frequency magnetic field to heat up nearby cells. For this purpose, it is most important to fine-tune the magnetic properties of the MNPs to increase the SAR (Specific Absorption Rate) parameter and thus reduce the dose of the administered drug. This can be achieved by creating core/shell MNPs composed of magnetically hard and soft materials. In this study, we investigated core/shell nanoparticles composed of maghemite and cobalt ferrite with varying thicknesses of cobalt ferrite shell. The synthesis of these nanoparticles involved a modified co-precipitation reaction, followed by hydrothermal surface treatment. Our focus was on evaluating the efficacy of these nanoparticles in hyperthermia for potential medical applications. Our findings revealed that the thickness of the cobalt ferrite shell plays a crucial role in enhancing the SAR parameter in magnetic hyperthermia. Specifically, we found that the thin cobalt ferrite shell was more effective than thicker shells, highlighting the importance of nanoparticle design in optimizing their performance for medical applications.

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Exploring the Formation Mechanisms of CoO and CoFe₂O₄ Nanomaterials Through Time-Resolved Synchrotron Analysis

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Cobalt (II) oxide (CoO) is a research material of substantial significance, recognized for its intricate properties relevant to basic research and its role in sustainable applications such as catalysis, lithium-ion batteries, water splitting, and permanent magnets[1]–[3]. The polyol method has been shown to produce CoO aggregates of approximately 100 nm in diameter with high porosity, a desirable characteristic for catalytic uses[4]. In this study, we utilized in-situ synchrotron techniques (XRD and SAXS) alongside ex-situ experiments (EXAFS, TEM, FTIR, etc.) to elucidate the formation mechanism of CoO and other synthesis byproducts. Our approach enabled real-time observation of layered hydroxide intermediates preceding CoO formation, allowing for resolving the formation of the single layers and their subsequent stacking. Notably, substituting di-ethylene glycol with tetra-ethylene glycol revealed significant alterations in the mechanism and in remarkable advantages in the synthesis feasibility conditions. Additionally, these synchrotron techniques were applied to the synthesis of CoFe₂O₄, a key material in magnetism research. Combined time-resolved XRD and SAXS measurements allowed us to observe the emergence of growing nanometric objects (2 to 5 nm) associated with XRD peaks related to the formation of the first coordination polyhedral in the structure. These advancements will serve a better understanding of the synthetic mechanisms of nanomaterials, developing new tools to improve the design of nanomaterials synthesis.

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Poster Session



NANOMAGNETS DISPERSED IN IONIC LIQUID-BASED SOLVENTS FOR THERMOELECTRIC CONVERSION

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In the search of sustainable energy solutions, ferrofluids made of charged magnetic nanoparticles (NPs) dispersed in ionic liquid-based solvents are gaining attention for thermoelectric applications. In this study, three water-based ferrofluids with different mean NPs sizes were synthesized via coprecipitation. Subsequently, the NPs surfaces were modified to enable dispersion in ionic liquid-based solvents. The effects of NPs composition and size, ligand type, and solvent properties on colloidal stability were evaluated using DLS, and SAXS measurements. Results demonstrated stable dispersions across all NPs sizes and solvent compositions. Notably, smaller NPs aggregated into larger clusters but remained stable in water for over a year. For dispersions in non-aqueous solvents, phosphonic ligands provided effective stabilization regardless of carbon side-chain length, while sulfonic ligands failed to stabilize dispersions, diverging from previous studies on maghemite NPs [1]. This difference is likely due to the stronger binding affinity of phosphonic groups and the intrinsic properties of cobalt ferrite, including a higher Hamaker constant [2] and greater magnetic anisotropy. Additionally, compared to their aqueous dispersions, NPs clusters in non-aqueous solvents were significantly reduced in size, containing only a few particles per cluster. This reduction was achieved through low-pressure pumping to remove water, followed by a heating step at 150°C. Both steps altered the organization of the solid/liquid interface, resulting in an equilibrium state unattainable at room temperature.

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COMPUTATIONAL ANALYSIS OF HEXAVALENT CHROMIUM ADSORPTION

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This study explores the removal of ionic pollutants, specifically hexavalent chromium (Cr(VI)), from water using computational simulations with magnetic nanoparticles. Hexavalent chromium, a highly soluble and toxic contaminant, presents significant challenges for removal from aqueous solutions. This work simulates the adsorption efficiency of cobalt and iron oxide core-shell nanoparticles ($\text{CoFe}_2\text{O}_4@\gamma\text{-Fe}_2\text{O}_3$) using the Monte Carlo method and the Metropolis-Hastings algorithm. The simulation examines interactions between nanoparticles of varying sizes and chromate (CrO_4^{2-}) and sulfate (SO_4^{2-}) ions in a controlled system, with ion concentration profiles revealing how adsorption is influenced by particle size and the presence of competing ions. The simulation model is informed by experimental data from the article “*Core-shell bimagnetic nanoadsorbents for hexavalent chromium removal from aqueous solutions*”[1], integrating experimentally derived characterizations and initial parameters as inputs. Results indicate that larger nanoparticles achieve higher adsorption efficiencies, particularly with chromate ions. These findings underscore the potential of magnetic nanoparticles as an effective and selective solution for removing heavy metal pollutants from contaminated water.

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Colloidal Characterization of a Composite of Essential Oil and Laponite in Water-Based Dispersions

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Essential oils (EOs) are natural volatile oils derived from plants that are widely investigated due to their biochemical properties and potential for applications, especially in the pharmaceutical and biomedical industries. The molecules that compose EOs are highly susceptible to natural instability, which leads to rapid degradation under ambient conditions, and for such applications, the stability of these molecules is essential, since some molecules can deteriorate with bad storage. In this sense, a variety of materials have already been employed to encapsulate and stabilize the EOs, acting as a matrix to prevent the decomposition of these molecules and increase their usefulness. Smectite clays are a matrix option that have attracted industry interest because of their abundance, affordability, versatility, and biocompatibility. This is primarily due to their advantageous physical-chemical characteristics, which include their large surface area, ion exchange capacity, and surface charges. As an example of a synthetic clay, Laponite (Lap) demonstrates good potential for stabilizing EOs since these nanoparticles have high purity, are almost monodispersed in size, and have well-defined dimensions that make for good modeling. Furthermore, upon addition to water, Lap produces a stable colloidal dispersion with a known phase diagram. Hence, this work aims to connect the best of both materials by combining Lap and EOs in a colloidal dispersion in order to produce a composite that can properly store the EOs in an adequate system for controlled and efficient applications. In this study, experimental analyses, including Gas Chromatography Coupled to Mass Spectrometry (GC-MS), Dynamic light scattering (DLS), Zeta Potential (ZP), and Small Angle X-ray Scattering (SAXS), were employed to characterize this composite's properties.

Ferrofluids based on Co-Zn-Cu Mixed Ferrites Nanoparticles for Hyperthermia

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Abstract: Spinel ferrite nanoparticles are versatile materials that can be used in a wide range of areas. Aiming magnetohyperthermia applications, we present here the study of ferrofluids based on nanoparticles of mixed ferrite of cobalt, zinc, and copper, elaborated to finely tune magnetization and magnetic anisotropy of ferrite magnetic nanoparticles by varying the chemical composition. Indeed, such mixed ferrite nanoparticles could present enhanced magnetic properties for this purpose [1]. These NPs are obtained by hydrothermal coprecipitation in alkaline medium followed by a surface treatment that creates an iron-rich surface layer allowing their dispersions in acid medium [2]. The nanoparticle chemical composition has been determined by chemical analysis using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) and Energy Dispersive X-Ray Fluorescence Spectroscopy (EDX). This crossed analysis allows us to precisely determine the proportions of core and shell volumes and the stoichiometry of the core materials in all samples investigated here. The crystalline structure and the nanoparticle sizes were studied by using X-Ray Diffraction (XRD). Transmission Electron Microscopy (TEM) pictures show their morphology and allow a mean size determination, which well matches the one deduced from XRD analysis. An extensive magnetic characterization was carried out using a SQUID magnetometer. Low and high field (7 T) DC magnetization experiments as a function of the temperature were combined with hysteresis loop measurements to investigate the magnetic behavior of the samples. The dependence of the high field magnetization on temperature is explained within Bloch's law. From the blocking properties and the thermal dependence of the coercivity we extract the anisotropy constant for all investigated samples. The first results show that magnetization and anisotropy can be tuned by the core composition and the core/shell architecture. Additionally, the Specific Absorption Rate (SAR) has been initially measured in few samples showing rather high values when compared to the literature and the value increases with the addition of Zn and Co in the core composition.

Key-words: nanoparticles, mixed ferrites, ferrofluid.

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MAGNETIC, ELECTRICAL AND STRUCTURAL PROPERTIES OF Fe-DOPED ITO FILMS GROWN BY RF MAGNETRON SPUTTERING TECHNIQUE

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Nowadays, the fabrication of thin films of diluted magnetic semiconductors, such as transition metal-doped indium tin oxide (ITO), is of great interest in the area of optoelectronics and spintronics for the fabrication of new devices. In this work, we present the study of Fe-doped indium tin oxide thin films, obtained by RF magnetron sputtering technique, annealed at different temperatures in air atmosphere (400-800°C). The film thickness is about 850 nm, as obtained by transmittance measurements. Furthermore, X-ray diffraction patterns confirmed the formation of the bixbyite-type cubic phase, showing good diffusion Fe atom within the crystal lattice. Rietveld refinement showed that the unit cell volume of the Fe-doped ITO compound decreases with the increase of the annealing temperature suggesting the presence of mainly Fe³⁺ substituting In³⁺ ions. Hall effect measurements showed n-type carriers with a value of $\sim 10^{20}$ cm⁻³ for the 400°C annealed sample, that decreases as the annealing temperature increases. Also, a reduction of the electrical resistivity with the annealing temperature was determined, which is consistent with the presence of Fe³⁺ ions acting as p-type doping [1]. Magnetization measurements at 2K showed a dominant paramagnetic behavior. When the annealing temperature was increased, a reduction of the magnetic moment was observed up to annealing temperatures of 600°C and for higher annealing temperature the magnetic moment returns to increase, likely suggesting the valence state change of iron ions between Fe²⁺ and Fe³⁺. In addition, a weak ferromagnetic contribution was observed at room temperature, which can be related to the interaction of delocalized charge carriers and magnetic ions in the semiconducting matrix.

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EFFECTS OF TEMPERATURE ON THE ELECTRONIC AND RESISTIVE PROPERTIES OF THE ACTIVE LAYER IN ORGANIC SOLAR CELLS

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Organic solar cells are emerging technologies aimed at replacing the conventional silicon-based solar panel model, representing a sustainable and innovative development with unique characteristics such as flexibility, adhesion, low production cost, and versatile materials [1]. However, despite their great potential, the technology faces several challenges regarding stability, with the main factors being photodegradation, temperature, and humidity [2]. Temperature is a degradation mechanism that directly affects the material's structure, which, depending on its physicochemical properties, results in morphological changes in the film, altering its band structure and consequently its energy levels. The objective of this work is to analyze the thermal degradation of the material when subjected to constant thermal treatment in the absence of light, according to ISOS-D-2 [3]. For this work, the polymers P3HT and N2300 were used, along with the PCBM molecule. The selection was based on the donor-acceptor nature of the materials, where the polymers were synthesized in their pure form. Additionally, bulk heterojunction processes P3HT:N2300 and P3HT:PCBM were carried out to analyze the individual degradation processes and to evaluate whether the mixtures delayed degradation, comparing them with the new optoelectronic properties created. The Characterization was performed using UV-VIS spectroscopy and profilometry techniques. Thus, the variations in band gap, resistance, and material absorption as thermal degradation occurred were analyzed, demonstrating the importance of the heterojunction process in improving the optoelectronic and resistive properties of the materials.

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STUDY OF THE MAGNETIC, STRUCTURAL AND VIBRATIONAL PROPERTIES OF PVA COATED Fe₃O₄ NANOPARTICLES

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In order to minimize the loss of nonmagnetic degrading elements in photodegradation processes, nanomaterials with good response to external magnetic fields, such as magnetite nanoparticles can be included in the fabrication of multicomponent nanostructures. In this work, the synthesis and characterization of magnetite nanoparticles is present. The nanoparticles were synthesized via microwave route. After the synthesis, a part of the resulting sample was washed using ethanol, in order to eliminate impurities. The as-prepared and washed samples were characterized via XRD, Fourier transform infrared spectroscopy and magnetic measurements. The structural analyses confirmed the formation of the magnetite spinel phase in both compounds, as the main component. The average size of the nanoparticles was estimated, showing a decrease from 13 nm to 8 nm after washing, suggesting the removal of impurities and a possible chemical reaction that reduced the crystallite size. In the as-prepared sample, beside the magnetite phase, functional groups of NH, PVA and hematite are detected. After the washing process, a decrease in the NH and hematite groups was determined, indicating the effectiveness of washing in the removal of the residual compounds. 300 K magnetic measurements of both compounds showed a superparamagnetic behavior. The saturation magnetization of the washed sample was 63 emu/g. The analysis of the ZFC and FC curves of the as-prepared sample indicated presence of a blocking temperature at 17K, associated with the relaxation of weakly interacting particles. A peak at 119 and a shoulder at ~265 K, were assigned to the Verwey transition of magnetite and Morin transition of hematite. After the washing process, the peaks related to the Verwey and Morin transitions disappeared suggests modifications in the magnetic properties of the magnetite phase, likely due to the chemical reactions occurring during the washing process.

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SYNTHESIS OF AQUEOUS MAGNETIC FLUIDS VIA ONE-POT APPROACH COMBINING POLYOL AND MASSART'S METHOD

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Magnetic fluids (MFs) have been extensively studied in recent decades, and their intriguing physicochemical properties have directed attention towards various applications in science and engineering, such as diodes, cosmetics, and drug carriers¹. Due to their interesting magnetic properties, magnetic nanoparticles can be used for tumor treatment. It is noted that the use of nanotechnology in healthcare is increasing the need to produce more precise, biocompatible, and low-cost materials. Thus, this work aims to contribute to the understanding of the physicochemical phenomena involving magnetic nanoparticles. By combining two highly relevant methods to understand the morphology, composition, and properties, magnetic core/shell type nanoferrites (CoFe₂O₄) were obtained through the combination of two well-known methodologies: polyol and hydrothermal co-precipitation²⁻³. The nanoparticles were characterized by X-ray Diffraction, Transmission Electronic Microscopy, Atomic Absorption Spectroscopy, and SQUID to analyze their morphology, composition, specific properties, and magnetization respectively.

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PHOTOCATALYTIC ACTIVITY OF DIFFERENT DOPANT CONTENT OF Fe-DOPED ZnO NANOPARTICLES

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ZnO nanostructures is a good candidate for applications on photocatalytic degradation of water contaminants. The doping of ZnO matrix with magnetic elements could improve its photocatalytic response by modifying the band alignment. In this work, iron-doped zinc oxide nanoparticles synthesized by the polymeric precursor method are systematically studied. Iron ions can stabilize in two oxidation states (Fe^{2+} and Fe^{3+}), with different ionic radii, which can affect the resulting properties of the Fe-doped ZnO nanoparticles. The oxidation state of the iron ions in the doped samples was assessed by room temperature ^{57}Fe Mossbauer spectroscopy. Only an electrical quadruple doublet was observed in the spectra. Results indicate that the isomer shift (IS) increases with the iron content, while the quadrupole splitting (QS) presented a similar increase. The values of the IS and QS parameters indicate that for the lowering doping samples (<10%) the iron is in the 2+ valence state, meanwhile for higher contents, it starts to appear irons in 3+ valence states, which also increases the structural disorder [1]. To evaluate the effectiveness of employment of Fe-doped ZnO nanoparticles as photocatalysts, we used a water containing the organic dye Rodamine-B in a 3ppm solution and at $\text{pH} \sim 7$. Our results show a better performance of the nanoparticles with low iron content, with respect to the nanoparticles with higher iron content. It suggests that the iron valence states can be related to the photocatalytic action of the Fe-doped ZnO nanoparticles.

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STABILITY IN FLEXIBLE CsFA PEROVSKITE PHOTOVOLTAIC DEVICES UNDER DIFFERENT AMBIENT CONDITIONS

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Perovskite solar cells (PSCs) are a promising innovation in energy generation. However, low stability under environmental factors is the main challenge for application in photovoltaic solar cells [1]. PSCs offer high power conversion efficiency (PCE), low cost, and great versatility in terms of applications [1]. In 2012, Lee and collaborators observed that perovskite could absorb light, generate electron-hole pairs, and transport them without losses due to recombination [1]. According to the National Renewable Energy Laboratory (NREL), in 2023, PSCs achieved an efficiency of 26.1% [2], a significant mark considering that crystalline silicon solar cells, particularly silicon heterojunction structures, reached an efficiency of 27.1% in the same year [2]. Despite their potential, PSCs still suffer from low durability. These cells are sensitive to environmental factors; oxygen, light, humidity, and temperature cause degradation after a short period of use. Many studies are being conducted to improve the stability of PSCs. This study aims to investigate the stability of perovskite films deposited on a flexible substrate under different degradation conditions over time. For this purpose, we employed the PET/ITO/NiOX/CsFA structure and evaluated physical stress conditions, such as temperature, light exposure, and mechanical flexibility, as well as chemical stress, humidity and water exposure. For this we use spectroscopic (UV-Vis, XPS), structural (XRD), morphological (AFM and SEM), and magnetic (SQUID) techniques for correlate stability with light, humidity, and temperature. Initial results show changes in the band gap energy when the material is exposed to temperatures based on the ISOS protocol [3].

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THERMAL DEPENDENCE AND SURFACE EFFECTS OF ANISOTROPY OF FERRIMAGNETIC COBALT NANOPARTICLES

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Improving the understanding of magnetic properties in nanostructured materials has been a great area of interest in materials exploration because of the advanced technological applications. Particularly, magnetic nanoparticles (MNPs) based on ferrimagnetic materials, such as spinel ferrites, have emerged as noteworthy candidates due to their tunable magnetic properties achievable through chemical composition and crystalline structure variations. This study delves into the thermal dependencies of saturation magnetization and anisotropy constant in ferrofluid samples based on size-distributed core-shell $\text{CoFe}_2\text{O}_4@ \gamma\text{-Fe}_2\text{O}_3$ NPs synthesized via hydrothermal coprecipitation in an alkaline medium. The NP sizes were controlled by modifying the synthesis medium. Subsequent hydrothermal surface treatment with $\text{Fe}(\text{NO}_3)_3$ produced the maghemite shell. Characterization of chemical, structural, and morphological properties was carried out using Atomic Absorption Spectroscopy, X-ray diffraction, and Transmission Electron Microscopy. Magnetic characterization was done measuring magnetization curves as a function of temperature. The ferrofluid samples were investigated, and we determined saturation magnetization and anisotropy constant values obtained by calculations involving the closure fields (H_{irr}) from hysteresis loops on Stoner-Wohlfarth model (S-W), and anisotropy fields (H_k) from the first magnetization curves, using the Law of Approach to Saturation (LAS)[1], comparing with the one obtained from the coercive field using a model based on S-W's [2,3] that considers size distribution and temperature dependence of magnetization and anisotropy constants, which influence the transition from blocked to superparamagnetic (SPM) states, providing meaningful insights into distinct sources of magnetic anisotropy arising from the ordered core and disordered shell, along with their temperature dependencies. The comparison between the different techniques helps to shed light on the magnetization processes and the role of surface spins on the magnetic properties in each field regime.

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SERS OF NATURAL LIPID-BASED NANOCARRIERS WITH RHODAMINE 6G AND CURCUMIN

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The formulation of nanostructured lipid carriers (NLC) with natural oils offers an optimal alternative for the controlled release of drugs in medical treatments and the reduction of the toxicity of organic compounds in clinical analysis [1]. Rhodamine 6G, a toxic organic compound used in clinical studies as a fluorescent marker for oncological treatments [2] and curcumin, a bioactive compound used for anti-inflammatory and anti-carcinogenic treatments [3], were both encapsulated in NLCs. The NLCs were formulated using natural lipids (palm kernel oil and murumuru butter) and the surfactant Kolliphor® HS at concentrations of 1.72×10^{-4} M for Rhodamine 6G and 9.64×10^{-4} M for curcumin. Optical and colloidal stability were analyzed by fluorescence and UV-vis spectroscopy, as well as dynamic light scattering (DLS) at intervals of 1, 2, and 3 months. Analysis by transmission electron microscopy (TEM) indicates NLCs with a quasi-spherical morphology and circular equivalent diameter around 70 nm (rhodamine-loaded) and 80 nm (curcumin-loaded); considering the specific compounds and the lipid matrix used. The interaction between the Rhodamine 6G and curcumin molecules with the lipid matrix were investigated using Fourier transform infrared spectroscopy (FTIR) and surface-enhanced Raman spectroscopy (SERS), employing a silver nanostructure substrate [4]. Changes in the intensities and energies of vibrational modes suggest that the presence of lipid matrix stabilizes the system through interactions of the Rhodamine 6G and curcumin molecules with the ester carbonyl groups of the lipid hydrocarbon chains.

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Impact of APTES ligand on zirconia nanocrystals and their colloidal stabilization in water

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Zirconia nanocrystals have been applied for several technological purposes, such as catalysis and nanocoating.[1] They often require colloidal stability in water or specific functional groups. The ligand 3-aminopropyltriethoxysilane (APTES) tightly anchors silane groups on zirconia surfaces, facilitating functionalization through the presence of reactive amino groups in its tail.[2,3] This work demonstrates and compares the ligand exchange reaction with APTES. Two functionalization routes were applied: one conducted via a one-pot strategy and the other performed using a solvent-based method under low-temperature conditions. Thermogravimetric, infrared, and elemental analyses provide quantitative and qualitative data on the presence of native and APTES ligands. The presence of native ligands is more evident in the one-pot method. There are more nitrogen groups per gram of nanoparticle (NP) (mmol N/g NP) in the solvent-based method than in the one-pot strategy, around 1.8 and 0.6 (mmol N/g NP) from elemental analysis, and 2.4 and 1.3 (mmol N/g NP) from thermogravimetric analysis, respectively. Furthermore, DLS and zeta-potential analyses with varying pH in water indicate an increase in the average size distribution above pH 5, due to nanocrystal aggregation and changes in surface charge, associated with amino group protonation. This behavior of the nanocrystals depends on the ligand composition and concentration on the surface. This study contributes to a better understanding of ZrO₂ nanoparticle modification and behavior, as colloidal stability in water is improved under acidic pH conditions and depends on the number of exchanged ligands. This is a fundamental step in the application of zirconia nanocrystals and in the design of ligand exchange procedures.

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