3NANO 2019

SCIENCE
TECHNOLOGY
BIOTECHNOLOGY

5TH International Conference on Nanoscience, Nanotechnology and Nanobiotechnology

ABSTRACTS BOOK

5th International Conference on Nanoscience,
Nanotechnology and Nanobiotechnology
Brasília, 8th – 12th December

FINATEC
UNIVERSIDADE DE BRASÍLIA

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SUN (12/08)	MON (12/09)	TUE (12/10)	WED (12/11)	THU (12/12)
	08:00 – 09:00 **Registration**		9:00 **IT 19** *D. Ugarte* 09:30 **IT 20** *G. M. Azevedo* *Chairperson: Y. Raikher*	9:00 **IT 29** *A. Cebers* 09:30 **IT 30** *J. Restrepo* *Chairperson: K. Trohidou*
	9:00 **Opening Session** 09:30 **IT 1** *A. Fazzio* *Chairperson: A. F. C. Campos*	9:00 **IT 10** *D. Fiorani* 09:30 **IT 11** *K. Trohidou* *Chairperson: J. Depeyrot*		
	10:00 – 10:30 **Coffee break**			
	10:30 **IT 2** Y. Raikher 11:00 **OC 1** *A. Amirov* 11:15 **OC 2** *B. C. da Silva* 11:30 **IT 3** *S. Lira* 12:00 **Flash Poster 1** *Chairperson: R. Perzynski*	10:30 **IT 12** *M. Rivas* 11:00 **OC 5** *T. Fiuza* 11:15 **OC 6** *L. Michels* 11:30 **IT 13** *T. del Rosso* 12:00 **Flash Poster 2** *Chairperson: A. Fazzio*	10:30 **IT 21** *E. Dubois* 11:00 **OC 11** *B. R. Salles* 11:15 **OC 12** *J. J. Atoche* 11:30 **IT 22** *V. Peyre* 12:00 **OC 13** *M. Chand* *Chairperson: R. Aquino*	10:30 **IT 31** *R. Brayner* 11:00 **IT 32** *A. F. C. Campos* *Chairperson: M. Rivas* 11:30 **Closing Session**
	12:15 – 14:00 **Lunch**			
	14:00 **IT 4** *A. M. F. Neto* 14:30 **OC 3** *M. P. da Silva* 14:45 **OC 4** *L. Scalvi* 15:00 **IT 5** *R. Perzynski* 15:30 **IT 6** *J. Wells* *Chairperson: M. Novak*	14:00 **IT 14** *L. Paterno* 14:30 **OC 7** *F. Mammeri* 14:45 **OC 8** *C. A. M. Vieira* 15:00 **OC 9** *L. Chaperman* 15:15 **OC 10** *A. Ghosh* 15:30 **IT 15** *S. Nakamae* *Chairperson: A. M. F. Neto*	14:00 **IT 23** *M. Novak* 14:30 **OC 14** *G. Gomide* 14:45 **OC 15** *F. G. da Silva* 15:00 **IT 24** *J. Geshev* 15:30 **IT 25** *F. Oliveira* *Chairperson: D. Ugarte*	
	16:00 – 16:30 **Coffee Break**			
18:00 – 20:00 **Registration**	16:30 **IT 7** *S. Ammar-Merah* 17:00 **IT 8** *R. Zysler* 17:30 **IT 9** *A. López-Ortega* *Chairperson: D. Fiorani*	16:30 **IT 16** *A. Bakuzis* 17:00 **IT 17** *G. Goya* *Chairperson: S. Ammar*	16:30 **IT 26** *S. Cassaignon* 17:00 **IT 27** *V. Rodionova* 17:30 **IT 28** *D. Peddis* *Chairperson: S. Nakamae*	
	Free	*Free* 20:00 **Conference Dinner**	18:00 – 20:00 **Poster Session**	

	Sunday – 08/12/2019
18:00	***Registration***
	Monday – 09/12/2019
9:00	***Opening Session***
Chairperson: A.F.C.Campos	
9:30	**IT 1 – A. Fazzio – Brazilian Nanotechnology National Laboratory (LNNano), Brazil** Towards Realistic Amorphous Topological Insulators
	10:00 – 10:30 Coffee break
Chairperson: R. Perzynski	
10:30	**IT 2 – Y. Raikher –Russian Academy of Science - Russia** Magnetoactive elastomers of mixed content: magnetic interaction of the filler particles
11:00	**OC 1 – A. Amirov –Immanuel Kant Baltic Federal University - Russia** Multiferroic Polymer Composite Based on Heusler-Type Magnetic Microwires with Combined Magnetocaloric and Magnetoelectric Effects
11:15	**OC 2 – B. C. da Silva – Institute of Physics "Gleb Wataghin" - Brazil.** Gallium Phosphide Nanowires: Epitaxial Growth and Optical Properties
11:30	**IT 3 – S. Lira – Universidade Federal de Alagoas, Maceió - Brasil** Nonequilibrium thermodynamics of a trapped nanoparticle in high vacuum
12:00	**Flash Poster 1**
	12 :15 – 14 :00 Lunch
Chairperson: M. Novak	
14:00	**IT 4 – A. M. F. Neto – Institute of Physics, University of São Paulo - Brazil** Influence of magnetic field on the two-photon absorption and hyper-Rayleigh scattering of manganese-zinc ferrite (MZ) nanoparticles
14:30	**OC 3 – M. P. da Silva - Faculdade UnB de Planaltina, UnB - Brazil** Synthesis and characterization of GO-H_3BO_3 composite for single sensor impedimetric olfaction.
14:45	**OC 4 – L. Scalvi - UNESP – Brazil** Transient Decay of Photoinduced Current in the Heterostructure GaAs/SnO_2 with Nanostructured Semiconductor Oxide Top Layer
15:00	**IT 5 – R. Perzynski Sorbonne Univ. CNRS, PHENIX Paris - France** Thermodiffusion probing of ferrofluids in ionic liquids
15:30	**IT 6 – J. Wells - University of Science and Technology - Norway** The electronic bandstructure of atomically sharp dopant structures in silicon
	16:00 – 16:30 **Coffee break**
Chairperson: D. Fiorani	
16:30	**IT 7 – S. Ammar-Merah - Université de Paris, ITODYS - France.** About the Exchange-Bias Feature in Magnetically Contrasted Oxide-Based Spsed Nanoconsolidates

17:00	**IT 8 – R. Zysler - Centro Atómico Bariloche - Argentina** Controlling the Dominant Magnetic Relaxation Mechanisms through the Shell Composition of Bi-Magnetic Core-Shell $Fe_3O_4/Zn_xCo_{1-x}Fe_2O_4$ Nanoparticles
17:30	**IT 9 – A. López-Ortega - Universidad de Castilla-La Mancha - Spain** Strongly Exchange Coupled Core|Shell Nanoparticles with High Magnetic Anisotropy: A Strategy Toward Rare-Earth-Free Permanent Magnets
Tuesday 10/12/2019	
Chairperson: J.Depeyrot	
9:00	**IT 10 – D. Fiorani - Istituto di Struttura della Materia - Italy** Surface Coating Effects on The Magnetic Properties of Spinel Ferrites Nanoparticles
9:30	**IT 11 – K. Trohidou - Institute of Nanoscience and Nanotechnology - Greece** Magnetic behavior of binary assemblies of nanoparticles
10:00 – 10:30 Coffee break	
Chairperson: A. Fazzio	
10:30	**IT 12 – F. Messina - Università degli Studi di Palermo - Italy** Towards a thorough understanding of the photophysics of Carbon Nanodots - Paving the way to fully harness their potential in photo-nano-technologies
11:00	**OC 5 – T. Fiuza - Instituto de Física, Universidade de Brasília, Brazil** Nanoscale Investigation on the Stability of Carbon Nanodots Aqueous Dispersions
11:15	**OC 6 – L. Michels - University of Science and Technology - Norway** Water vapor diffusive transport in a smectite clay: Cationic control of normal versus anomalous diffusion
11:30	**IT 13 – T. del Rosso - Pontifícia Universidade Católica do Rio de Janeiro - Brazil** The carbon beyond the gold: a novel insight on the potentialities of ligand-free pulsed laser ablation of a gold target in water
12:00	**Flash Poster 2**
12:15 – 14:00 **Lunch**	
Chairperson: A. M. F. Neto	
14:00	**IT 14 – L. Paterno - Universidade de Brasília - Brazil** Electronic tongue: multisensor array for classification and quantitative analysis of liquid samples
14:30	**OC 7 – F. Mammeri - Université de Paris, ITODYS - France** Preparation of Hybrid PVDF-$COFE_2O_4$ Self-Standing Films for Magnetoelectric Applications: Is There a Sustainable Alternative to the use of Dimethylformamide?
14:45	**OC 8 – C. A. M. Vieira - - Instituto de Física, Universidade de Brasília, Brazil** Interparticle Interactions and Magnetic Blocking Properties of Fine Ferrite Nanoparticles
15:00	**OC 9 – L. Chaperman - Université Paris Diderot - France** TiO_2-based photoanodes for solar-powered Hydrogen generation: controlled surface oxidation as a soft chemistry path towards water-splitting
15:15	**OC 10 – A. Ghosh - University of Ceará, Fortaleza - Brazil** One-Pot Synthesis of Titanate-Titania Nanoheterostructure: Synergistic Modification of Band Structure and Surface Property for Improved Photocatalytic Application
15:30	**IT 15 – S. Nakamae - Université Paris Saclay - France** Recent Advancements in Nano-Fluid Thermoelectric Research
16:00 – 16:30 **Coffee break**	

Chairperson: S. Ammar	
16:30	**IT 16 – A. Bakuzis - Universidade Federal de Goiás, Goiânia - Brazil** Can Infrared Surface Temperature Measurements Be Used To Determine Intratumoral Thermal Dose During Magnetic Nanoparticle Hyperthermia
17:00	**IT 17 – G. Goya - Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza - Spain** Low-dimensional assemblies of magnetic nanoparticles improve in vitro heating power through dipolar Interactions
17:30	**IT 18 – M. Rivas - University of Oviedo - Spain** Magnetoimmunoassays for health and healthy wine
	20:00 **Conference Dinner**
	Wednesday - 11/12/2019
Chairperson: Y.Raikher	
9:00	**IT 19 – D. Ugarte - Universidade Estadual de Campinas - Brazil** Detailed Structural Characterization of Nanomaterials by Precession Electron Diffraction
9:30	**IT 20 – G. M. Azevedo – Universidade Federal do Rio Grande do Sul - Brazil** Decreasing Nanocrystal Structural Disorder by Ligand Exchange: An Experimental and Theoretical Analysis
	10:00 – 10:30 **Coffee break**
Chairperson: R. Aquino	
10:30	**IT 21 – E. Dubois – Sorbonne Univ. CNRS, PHENIX - France** Ferrofluids in ionic liquids: high temperature study
11:00	**OC 11 – B. R. Salles – Instituto de Física, Universidade Federal do Rio de Janeiro - Brazil** Magnetic Properties of Core-Shell Fe-Pt Nanoparticles in Ionic Liquids
11:15	**OC 12 – J. J. Atoche – University of Brasilia - Brazil** Synthesis and Characterization of Core-Shell ($Au@Fe_3O_4$) Nanostructure
11:30	**IT 22 – V. Peyre - PHENIX, Sorbonne Universités, UPMC Univ Paris 06 - France** Colloidal materials in ionic liquids: influence of ionic and water content on dispersions stability
12:00	**OC 13 – M. Chand - Faculty of Planaltina Campus, University of Brasilia - Brazil** Magnetorheological studies on aligned CNTs dispersed in magnetic fluid
	12:15 – 14:00 **Lunch**
Chairperson: D. Ugarte	
14:00	**IT 23 – M. Novak - Universidade Federal do Rio de Janeiro - Brazil** Dynamics of highly anisotropic magnetic chains
14:30	**OC 14 – G. Gomide - Instituto de Física, Universidade de Brasília, Brazil** Thermal Dependence of Coercivity, Irreversibility and Magnetic Anisotropy in Ferrimagnetic Nanoparticles
14:45	**OC 15 – F.G. da Silva - Faculdade UnB Planaltina, Universidade de Brasília - Brazil** Magnetic irreversibility and saturation criteria in ultrasmall bi-magnetic nanoparticles
15:00	**IT 24– J. Geshev - Instituto de Física, URFGS - Brazil** Discerning Bulk from Interface Interactions in Magnetic Nanostructures

15:30	**IT 25 – F. Oliveira - University of Brasilia - Brazil** The Kubo Fluctuation-Dissipation Theorem
	16:00 – 16:30 **Coffee break**
Chairperson: S. Nakamae	
16:30	**IT 26 – S. Cassaignon - Sorbonne University, CNRS - France** From Synthesis to Applications: Design of Nanomaterials for Property Control
17:00	**IT 27 – V. Rodionova - Immanuel Kant Baltic Federal University - Russia** Amorphous, Partially Crystalline and Crystalline Magnetic Microwires: From Fabrication and Properties to Practical Applications
17:30	**IT 28 – D. Peddis - Istituto di Struttura della Materia –Italy** Design advanced magnetic nanocomposites based on transition metal oxides
	18:00 – 20:00 **Poster Session**
	Thursday -12/12/2019
Chairperson: K. Trohidou	
9:00	**IT 29 – A. Cebers - University of Latvia, Riga - Latvia** Dynamics of Flexible Ferromagnetic Filaments
9:30	**IT 30 – J. Restrepo - Universidad de Antioquia - Colombia** Dual Reversal Modes by Helicity Control in Ferromagnetic Nanotubes: Monte Carlo Simulation and Micromagnetic Approach
	10:00 – 10:30 **Coffee break**
Chairperson: F. Messina	
10:30	**IT 31 – R. Brayner - Université de Paris, ITODYS - France** Alginate@PLGA nanocomposite beads for the prolonged delivery of haloperidol antipsychotic to the brain via an oral route
11:00	**IT 32 – A. F. C. Campos - Faculty UnB – Planaltina, University of Brasília - Brazil** Application of core@shell based magnetic nanoadsorbents for water remediation
	11:30 Closing Session

	Poster Session
P01	**A. Omelyanchik – Immanuel Kant Baltic Federal University, Kaliningrad, Russia** Magnetic and Structural Properties of Cobalt Ferrite Nanoparticles Doped with Zinc and Nickel
P02	**A. Q. Sena –University of Brasilia - Brazil** Tuning Long-Range Functionals for Determining Reorganization Energies of Photosynthetic Systems
P03	**A. A. A. M. Guerra – University of Brasilia - Brazil** Adsorptive Removal of Phosphorus by Core-Shell Bimagnetic Nanoparticles
P04	**A. S. Aguiar - University of Brasilia - Brazil** Synthesis of Magnetic Nanoparticles Embedded in a Laponite Dispersion

P05	**A. P Maciel - UnB – Planaltina Campus, University of Brasilia - Brazil** L-Lysine Coated Magnetic Nanoparticles for ASA Removal from Aqueous Solutions
P06	**B. C. C. Pereira - University of Brasilia - Brazil** Investigation of the Magnetic Properties of Cobalt, Zinc and Copper Mixed Ferrite Nanoparticles
P07	**B. C. C. de Almeida – University of Brasilia - Brazil** On Water Clusters Cis-Trans Structures Properties
P08	**C. J. Domingos da Cruz – University of Brasilia - Brazil** Magneto Hyperthermia of Core/Shell (γ-Fe_2O_3@$CoFe_2O_4$) Nanoparticles: The Effect of Shell Thickness
P09	**C. Amaral - Department of Electrical Engineering, University of Brasilia - Brazil** Towards the Contact-Free Measurement of Large Sheet Resistances
P10	**C. F. Bueno - São Paulo State University - Brazil** Study of SnO Thin Films Grown by MBE for SnO/SnO_2 *p-n* Junction Formation
P11	**D. Liguori - University of Brasilia, Brasilia – Brazil** Organoclay Preparation and Characterization Aiming Wastewater Treatment Applications
P12	**D. Neves - Department of Electrical Engineering, University of Brasilia, Brasilia – Brazil** Quantum Phenomena in Nanoscale Transistors with Multiple Gates
P13	**E. Valamontes - University of West Attica - Greece** Size and Shape Effects on the Hyperthermia Performance of Bi-Magnetic Core / Shell Nanoparticles
P14	**F. Mammeri - Université de Paris, ITODYS, Paris - France** Wrinkling Evolution of Tantalum Films Sputter Deposited on PDMS Substrate Under Uniaxial Strain
P15	**F. M. Carvalho - Physics Institute, University of Brasilia - Brazil** Modeling Exciton Diffusion in Crystalline Chromophore Assemblies
P16	**F. M. Carvalho - Physics Institute, University of Brasilia - Brazil** Virtual Screening and Quantum-Chemical Study of the Prediction pKa's Sulfa-like Compounds
P17	**F. L. O. Paula - Physics Institute, University of Brasilia, Brasilia, Brazil** Study of Nanoparticle Structure on Ph-Dependent Ferrofluid Phase Transition by Means of Monte Carlo Simulation
P18	**F. T. Bueno - Physics Institute, University of Brasilia - Brazil** Exciton Density Effects in Organic Materials: Diffusion Length, Lifetime and Quantum Efficiency
P19	**G. H. L. Dias - Physics Institute, University of Brasilia - Brazil** Dynamics and Rovibrational Spectroscopy of Weakly Bonded Complexes
P20	**G. Niraula - Department of Physics, Federal University of Maranhão - Brazil** Role of Size, Morphology, Surface Composition on Magnetic Vortex State and Hyperthermia Properties of Iron Oxide Nanoparticles
P21	**G. G. Silva -LNAA, - UnB – Planaltina Campus, University of Brasilia - Brazil** Dispersion of $CoFe_2O_4$ Functionalized Nanoferrite into a Deep Eutectic Solvent
P22	**H. Oliveira -LNAA, - UnB – Planaltina Campus, University of Brasilia - Brazil** Removal of As(V) from Aqueous Solutions Using Core@Shell Bimagnetic Nanoadsorbents
P23	**H. N. Coutinho – Chemistry Institute, University of Brasilia - Brazil** A DFT Study of C18O2 Heterofullerene Isomers
P24	**I. G. Ribeiro - University of Brasilia - Brazil** Singlet Exciton Diffusion Length In Benzodiindolizines Derivatives
P25	**I. P. de Siqueira - University of Brasilia - Brazil** Understanding the Importance of Chlorophylls, Carotenoids, and Xanthophylls in Photosynthesis by the Förster Resonance Energy Transfer Study
P26	**J. F. A. Carneiro - University of Brasilia, *Campus* Planaltina, Brazil** A Comparative Study of Protocols for Exciton Diffusion Length Estimation
P27	**J. H. D. Florentino - Complex Fluids Group, University of Brasilia, *Campus* Planaltina - Brazil** Polyol Sinthesis Conditions for Cobalt Ferrite Nano-Objects and Ferrofluid Elaboration
P28	**J. Ricardo - Instituto de Física, Universidade de Brasília - Brazil** Using Raman Spectroscopy for Identification of Three Microalgae Species
P29	**L. Born - University of Brasilia, Brasilia, Distrito Federal - Brazil** Energetic and Vibrational Disorders on Exciton Dynamics in Organic Thin Films
P30	**L. Born - University of Brasilia, Brasilia, Distrito Federal - Brazil** The Effects of Vibrational Disorder in Singlet Exciton Diffusion in Organic Compounds
P31	**L. Scalvi - Department of Physics, São Paulo State University - Brazil** Investigation of Photo-Induced Electrical Response Under Gas Incidence in SnO_2: 1%at Er^{3+} Based Thin Film Samples
P32	**L. S. R. de Paiva - University of Brasilia, Brasilia, Distrito Federal - Brazil** Oligomer Size Effects on Exciton Diffusion Length
P33	**L. B. de Paula - Department of Chemistry, University of São Paulo - Brazil** Designing Tumor Spheroids Technologies for 3D in Vitro Brain Cancer Model for Nanomedicine

	Screening
P34	**L. L. e Castro - Physics Institute, University of Brasilia, Brasilia - Brazil** Improvements of DLVO Theory Applied to Magnetic Nanoparticle Interaction in Ferrofluids
P35	**L. G. Paterno – Chemistry Institute, University of Brasilia - Brazil** SERS Active Substrates Made by Photocatalytic Deposition of Ag Nanoparticles
P36	**L. T. M. de Sousa - Chemistry Institute, University of Brasilia - Brasil** Molecular Dynamics of Pure Liquids - Octane, Nonane and Benzonitrile Benchmark of the OPLS Force Field
P37	**L. H. H. I. Cavamura - University of Brasilia – Brazil** Impact of Tuning the Long Range Parameter on Exciton Diffusion Length Predictions in Organic Systems
P38	**M. G. Viana – Federal Institute of Education, Science and Tecnology of Piauí, Campus Oeiras - Brazil** Investigation of the Magnetic Properties of $CoFe_2O_4$@γ-Fe_2O_3 Core/Shell Nanoparticles
P39	**M. Zavarize - Institute of Physics “Gleb Wataghin”, University of Campinas, Campinas - Brazil** Exploring Mg and Bi as Catalysts for Wurzite InP Nanowire Growth
P40	**M. Montero-Muñoz - Institute of Physics, University of Brasilia - Brazil** Morphology-Design of ZnO Nanostructures and its Correlation with the Structural, Vibrational and Optical Properties
P41	**M. Montero-Muñoz - Institute of Physics, University of Brasilia - Brazil** Atomic-Level and Electronic Structure Insight of Co^{2+}-Doped ZNo Nanocrystals
P42	**M. C. Mathpal - Institute of Physics, University of Brasilia – Brazil** Direct Realization of Microstructure Changes in Some Metal Oxide Nanostructures by Raman Spectroscopy and Electron Microscopy
P43	**P. F. Reis - University of Brasilia, Planaltina Campus, - Brazil** Removal of Lead from Aqueous Solutions by Cysteine-Coated Magnetic Nanoparticles
P44	**P. R. Teixeira - University of Brasilia, Planaltina Campus, - Brazil** Electrochemical Detection of Triclosan in Tooth Paste and Lake Water Samples by Means of Gold Nanoparticle-Polyionic Liquid Nanocomposite Electrode
P45	**R. Vasconcelos - Institute of Physics, University of Brasilia, Campus Darcy Ribeiro – Brazil** Control of Monolayer $MgCl_2$ Electronic Properties Through Substitutional Doping of Nonmetals and Transition Metals
P46	**R. F. C. B. Pedrosa - University of Brasilia, *Campus* Planaltina - Brazil** Graphene/(di-methyl di-dodecyl quartenary ammonium) LBL for Non-Specific Impedimetric Sensor
P47	**R. P. Muniz - Laboratório de Nanociência Ambiental e Aplicada-LNAA, University of Brasilia - Brazil** Use of the Ionic Strength to Improve the Colloidal State of Aqueous Magnetic Fluids
P48	**S. L. P. da Silva – Chemistry Institute, University of Brasilia - Brazil** Photochemical Synthesis of Silver Nanoparticles Stabilized by Graphene Oxide-Poly(Ethylene Imine) Nanocomposite
P49	**T. Q. Muniz – University of Brasilia – Brazil** Effect of Shell Thickness on the Magnetic Properties of $CoFe_2O_4$@γ-Fe_2O_3 Core/Shell Nanoparticles
P50	**T. Fiuza – University of Brasila - Brazil** Anisotropy of the Thermodiffusion Under Magnetic Field in Ionic Liquid Based Ferrofluid
P51	**T. S. A. Cassiano – University of Brasilia – Brazil** A Monotonic Gap Tunning Through Changes in Aromaticity for the Cove-Type Graphene Nanoribbon
P52	**Yu. L. Raikher - Institute of Continuous Media Mechanics, Russian Academy of Science - Russia** Modeling of the Field-Induced Response of a Magnetic Polymersome
P53	**T. F. Santana – Faculty of Gama, University of Brasilia – Brazil** Liposomes Use in Diabetic Wounds Treatment: A Systematic Review

INVITED TALKS

IT1

Towards Realistic Amorphous Topological Insulators

Marcio Costa[1,2], Gabriel R. Schleder[2,] M. B Nardelli[3,4], Caio Lewenkopf[5], and Adalberto Fazzio[1]
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[2]*Center for Natural and Human Sciences, Federal University of ABC (UFABC), 09210-580, Santo André, São Paulo, Brazil*
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The quantum Hall effect (QHE) initiated the era of topological states of matter. The hallmark of QHE is the existence of a quantized Hall conductivity, first observed in a 2D electron gas under a strong magnetic field. Inspired by the works of Thouless and Haldane, Kane and Mele showed how a quantized conductance can arise for a class of Hamiltonian systems in the presence of spin-orbit coupling (SOC) without magnetic fields, the so called quantum spin Hall (QSH) effect. The QSH phase is characterized by the existence of metallic edge states protected against disorder by time-reversal symmetry (*T*). A fundamental issue is whether a topological insulator protected by time-reversal is robust enough under a transformation to an amorphous state. The key role of translational symmetries in building the theory of topological insulators raises the question: to what extent is translational symmetry necessary for a topological state to retain its properties?

A non-trivial topological phase in an amorphous system was recently reported in a two- dimensional lattice of random set points simulating an amorphous Chern insulator [1]. However, until now, topological phases in amorphous systems have only been reported for simple lattice models or nonmaterial specific systems.

Using ab initio calculations (DFT) we show that two-dimensional amorphous materials can also display topological insulator properties. More specifically, we present a realistic state-of-the-art study of the electronic and transport properties of amorphous bismuthene systems, showing that these materials are topological insulators. Our study is motivated by the recent synthesis of suche material on a SiC substrate[2]. These systems are characterized by the topological index Z2 = 1 and bulk-edge duality, and their linear conductance is quantized, G = 2e2/h, for Fermi energies within the topological gap. Our study opens the path to the experimental and theoretical investigation of amorphous topological insulator materials.

[1] Agarwala, A.; Shenoy, V. B. Phys. Rev. Lett. 2017, **118**, 236402.
[2] Reis, F.; Li, G.; Dudy, L.; Bauern- feind, M.; Glass, S.; Hanke, W.; Thomale, R.; Schäfer, J.; Claessen, R. Science 2017, **357**, 287– 290

MAGNETOACTIVE ELASTOMERS OF MIXED CONTENT: MAGNETIC INTERACTION OF THE FILLER PARTICLES

O. V. Stolbov[1], T. I. Becker[2], D. Yu. Borin[3], K. Zimmermann[2], Yu. L. Raikher[1]
[1] Institute of Continuous Media Mechanics, Russian Academy of Science, Ural Branch, Perm, Russia
[2] Technical Mechanics Group, Technische Universität Ilmenau, Ilmenau, Germany
[3] Institute of Mechatronic Engineering, Technische Universität Dresden, Dresden, Germany

Magnetoactive elastomers of mixed content (MAE-MC) [1,2] are composites whose filler is a mixture of magnetically soft (MS) and hard (MH) microparticles. The macroscopic properties of MAE-MC differ greatly from that of usual MAE with only MS particles, and that is evidently due to the presence of the MH component. In particular, the magnetization response of the material, both in the field-free state and under the field by no means resembles any kind of superposition of the phase contributions. The surprising features of these very new (and practically very prospective) systems pose interesting theoretical challenges and require new theoretical models.

We show that to understand the magnetic behavior of a MAE-MC sample, one has to take into account the history of its magnetization and the two-fold effect of the presence of the MS particles which surround the MH ones in the elastomer matrix. On the one hand, the MS "shell" to some extent screens out the magnetic moments of the MH grains, but on the other hand, the MS particles work as mesoscopic flux-conducting bridges which enhance the strength of internal field in comparison with that of the externally applied one. The interplay of those two mechanisms, which, in turn, depend on the phase concentration, spatial distribution, applied field strength, etc. defines the magnetic characteristics that MAE-MC demonstrate in macroscopic experiments. Examples of measurements on real MAE-MC are given.

Support: OVS and YLR acknowledge RFBR grant 19-52-12045, TIB and KZ – DFG grant BE-6553/1-1.

[1] J. Linke, D. Borin, S. Odenbach, RSC Advances 6, 100407 (2016)
[2] G. Stepanov, D. Borin, A. Bakhtiiarov, P. Storozhenko, Smart Mater. Struct. 26, 035060 (2017)

IT3

Nonequilibrium thermodynamics of a trapped nanoparticle in high vacuum

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We perform an analytical study on the stochastic thermodynamics of a small classical particle trapped in a time-dependent single-well potential in the highly underdamped limit. It is shown that the nonequilibrium probability density function for the systems energy is a Maxwell-Boltzmann distribution (as in equilibrium)with a closed form time-dependent effective temperature and fractional degrees of freedom. We also find that the solvable model satisfies the Crooks fluctuation theorem, as expected. Moreover, we compute the average work in this isothermal process and characterize analytically the optimal protocol for minimum work. The optimal protocol presents an initial and final jump which correspond to adiabatic processes linked by a smooth exponential time-dependent part for all kinds of single-well potentials. Furthermore, we argue that this result connects two distinct relevant experimental setups for trapped nanoparticles, the levitated particle in a harmonic trap, and the free particle in a box, as they are limiting cases of the general single-well potential and display the time-dependent optimal protocols. Finally, we highlight the connection between our system and an equivalent model of a gas of Brownian particles.

[1] J. Gieseler, R. Quidant, C. Dellago, and L. Novotny, Nat. Nanotech. 9, 358 (2014).
[2] D. S. P. Salazar and S. A. Lira, J. Phys. A 49, 465001 (2016).
[3] D. S. P. Salazar and S. A. Lira, Phys. Rev. E 99, 062119 (2019).

IT4

Influence of magnetic field on the two-photon absorption and hyper-Rayleigh scattering of manganese-zinc ferrite (MZ) nanoparticles

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Colloidal solutions containing nanoparticles with distinct shapes (labeled as MZS, containing spherical nanoparticles, and MZC, composed of cubic NPs) were studied by means of the hyper-Rayleigh scattering (HRS) technique, allowing the determination of the optical second harmonic generation, β, by the Z-Scan (ZS) technique, for the determination of the two-photon absorption cross-section (σ_{2PA}). An external magnetic field was applied in order to orient the particles in solution, aligning the individual easy axis parallel to the external field. HRS and ZS experiments were performed with applied magnetic field both in the parallel configuration (where the incident laser beam polarization was parallel to the magnetic field) and in the perpendicular case (where the laser beam polarization and the magnetic field directions were orthogonal). The linear attenuation spectrum does not change regardless the field presence, indicating that the nanoparticles are being oriented but not forming structures big enough to scatter light. This interpretation was supported by the SAXS results, also measured in the presence of magnetic field, that demonstrates the formation of small chain-like aggregates, composed by few nanoparticles. Femtosecond transient absorption measurements revealed an ultrafast relaxation process containing at least two separated dynamical processes. The characteristic time of the fast component was $\tau^{\odot} = 0.9(1)$ ps for spherical nanoparticles and $\tau^{\boxdot} = 0.7(1)$ ps for the cubic ones, and has its origin in exciton-exciton annihilation, while the second one, much longer, may be related to the trapped electron on the conduction band. The hyperpolarizability of spherical nanoparticles in the absence of magnetic field was $\beta^{\odot} = 9.5(2) \times 10^{-28}$ cm^5/esu, while of cubic ones, $\beta^{\boxdot} = 7.8(1) \times 10^{-28}$ cm^5/esu. The difference on the value can be attributed to differences on the volume of nanoparticles as well as effects of a spin-disoriented shell, reducing the oriented average value of the hyperpolarizability of smaller nanoparticles. Optical second harmonic measured in the presence of external field in the parallel configuration presented an increase in value, that is, for spherical nanoparticles (MZS), $\beta^{\odot}_{\parallel} = 10.1(2) \times 10^{-28}$ cm^5/esu, and for MZC sample, $\beta^{\boxdot}_{\parallel} = 8.1(2) \times 10^{-28}$ cm^5/esu. On the other hand, a slight decrease on the hyperpolarizability was measured for experiments performed on the perpendicular configuration, $\beta^{\odot}_{\perp} = 9.3(3) \times 10^{-28}$ cm^5/esu for MZS and $\beta^{\boxdot}_{\perp} = 7.4(2) \times 10^{-28}$ cm^5/esu for the cubes. Therefore, the anisotropy in the first-order hyperpolarizability $\delta\beta = (\beta_{\parallel} - \beta_{\perp})/\beta_{\parallel}$ was determined as 8(3) % for spherical nanoparticles and 8(2) % for the cubes. The two-photon absorption cross-section in the absence of external magnetic field was measured as $\sigma^{\odot}_{2PA} = 17(1)$GM for spherical nanoparticles and $\sigma^{\boxdot}_{2PA} = 17(1)$ GM for the cubes, compatible within the experimental errors. For both studied nanoparticles, the 2PA cross-section measured in the parallel configuration presented an increment in the value, while in the perpendicular configuration, the measured value decreased when compared to H = 0. These experiments put in evidence the anisotropy in the nonlinear optical properties our ferrite nanoparticles, as well as the possibility of controlling the scattering of the generated second-harmonic and the two-photon absorption of colloidal solutions of magnetic nanoparticles by means of an external magnetic field.

FAPESP, CNPq, CAPES, INCT-FCx

IT5

Thermodiffusion probing of ferrofluids in ionic liquids

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Ionic liquids (ILs) are a wide class of solvents, purely constituted of ions, which can be liquid at room temperature. IL-based ferrofluids are new thermoelectric materials, versatile, cost-effective and non-toxic to assist the economically and environmentally sustainable energy transition [1]. A simple model-system of IL-based ferrofluid with citrate-coated maghemite nanoparticles (NPs) dispersed in ethylammonium nitrate [2,3] is first studied. Then more complex IL-based systems are investigated varying parameters such as IL-anions or -cations, NP coating and temperature (295K<T<473K) [4]. Their probing involves :

- Simultaneous Dynamic Light Scattering and Small Angle Neutron Scattering measurements, performed at LLB-Saclay-France to study the colloidal stability and the interparticle interaction in the dispersions as a function of T,
- Forced Rayleigh scattering [5,6,7] as a function of T to determine the NP diffusion coefficient and their Soret coefficient.

[1] B. Huang et al J. Chem. Phys. 143, 054902 (2015)
[2] M. Mamusa et al Soft Matter 10, 1097 (2014)
[3] K. Battacharya et al (submitted)
[4] J.C. Riedl et al (submitted)
[5] M. Kouyaté et al Phys. Chem. Chem. Phys. 21, 1895-1903 (2019)
[6] R. Cabreira-Gomes et al Phys. Chem. Chem. Phys., 20, 16402-16413 (2018)
[7] M. Sarkar et al EPJE 42,72 (2019)

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IT6

The electronic bandstructure of atomically sharp dopant structures in silicon

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Recently, it has become possible to control the placement of dopants in silicon with atomic precision, and this has given rise to a plethora of atomic scale and quantum proto-devices [1-3]. In this talk, I will present our ongoing work on understanding the electronic bandstructure of these dopant profiles in silicon.

Angle Resolved Photo-Electron Spectroscopy (ARPES) is the method of choice for observing the bandstructure, however observing the bandstructure of buried structures is extremely challenging. We have demonstrated that it is nonetheless possible to use ARPES to measure the bandstructure of dopant structures which have been created several nm beneath the surface [4]. It is also possible to see electron-phonon and electron-impurity interactions [5], quantum confinement of both the valence band and conduction band [6] and more. I will present these findings together with an overview of the current in understanding and controlling the electronic structure of dopant assemblies in semiconductors.

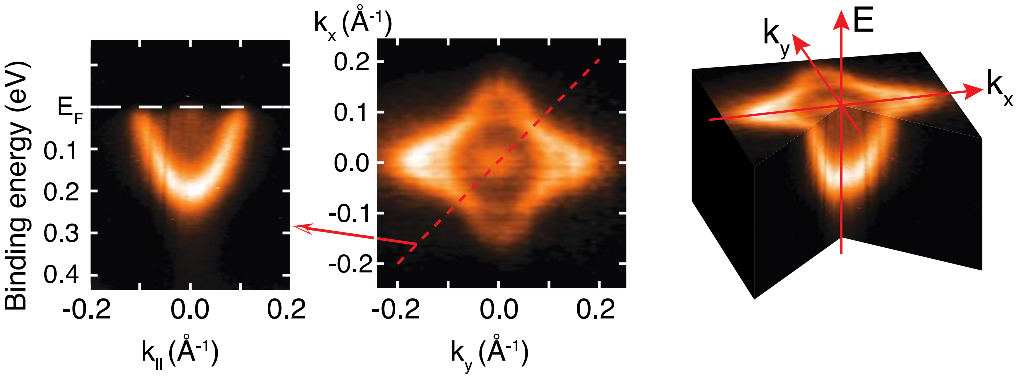

Figure: The measured electronic bandstructure of a 2D plane of dopants within a silicon host (so-called “delta-layer”) located several nm beneath the sample surface.

[1] Weber *et al.,* Science 335, 64 (2012)
[2] Zwanenburg *et al.*, Rev. Mod. Phys. 85:961 (2013).
[3] Watson *et al.*, Nature 555, 633 EP (2018)
[4] Miwa *et al*., Phys. Rev. Lett. 110:136801 (2013)
[5] Mazzola *et al.,* Appl. Phys. Lett. 104: 173108 (2014)
[6] Mazzola *et al.*, Phys. Rev. Lett. 120:046403 (2018)

IT7

ABOUT THE EXCHANGE-BIAS FEATURE IN MAGNETICALLY CONTRASTED OXIDE-BASED SPSED NANOCONSOLIDATES

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The combination of a ferro-, ferrimagnetic (F) with an antiferromagnetic (AF) material can lead to a spin exchange coupling known as “exchange bias” EB. This phenomenon is characterized by an asymmetric hysteresis loop and an enhanced coercive field [1]. To be most effective, this phenomenon requires nanostructures with maximum interface contact. For this reason, it is mainly focused on multilayers and nanoparticles (NPs) where the interface between the F and AF phases is easier to control. As a result, it is particularly active in the technological fields involving thin films and colloids, such as those of magnetic recording heads [2], magnetoresistive random access memories (MRRAM) [3], magnetic sensors [4] and high storage capacity magnetic recording media [5], for the former, and those of magnetic hyperthermia therapeutic fluids [6], for the later. Even so, it is hardly considered for applications involving bulk solids, regarding the technical difficulty of their processing. The emergence of Spark Plasma Sintering (SPS) technique has propelled a renewed interest on hetero-nanostructured consolidates, opening the way to the production of E-biased solids. Indeed, SPS operates at moderate temperatures for short period of times, favoring ultrafine grained and highly dense microstructures [7]. Under these conditions, the limits highlighted could be overcome and as pioneering research, we combined soft chemistry, the polyol process, and SPS in order to prepare such solids, starting from E-biased core-shell NPs or a mixture of F and AF NPs, and finding the best sintering conditions in order to promote large and highly criystallized interfaces. As a case study, we focused on F CoFe$_2$O$_4$ cobalt ferrite interfaced with AF NiO or CoO oxide, which exhibit interesting magnetic properties for the design of such solids and their characterization [8] within relatively easy-to-achieve operating conditions. Their respective ordering temperatures (800 vs. 525 and 290 K) as their magnetocrystalline anisotropy constants (1.20 vs. 0.01 and 3.00 MJ.m^{-3}) are significantly different, allowing an easy experimental evidence of EB at or below room temperature.

[1] J. Nogués et al., Phys. Rep. 422, 65 (2005).
[2] M.N. Baibich et al., Phys. Rev. Lett. 61, 2472 (1988) ; B. Dieny et al., Phys. Rev. B 43, 1297 (1991).
[3] S.M. Wu et al., Nat. Mater. 9, 756 (2010) ; S. Yuasa et al., MRS Bull. 43, 352 (2018).
[4] Y. Cheng et al., Phys. Lett. A 382, 3018 (2018) ; V. Apicella et al., Sens. Act. A 280, 475 (2018).
[5] V. Skumryev et al., Nature 423, 850 (2003).
[6] H. Khurshid et al., J. Appl. Phys. 117, 17A337 (2015).
[7] T. Gaudisson et al., J. Magn. Magn. Mater. 370, 87 (2014) ; T. Gaudisson et al., J. Magn. Magn. Mater. and 387, 90 (2015).
[8] G. Franceschin et al., Sci. Rep. (2019) *doi: 10.1038/s41598-019-50657-4*

IT8

CONTROLLING THE DOMINANT MAGNETIC RELAXATION MECHANISMS THROUGH THE SHELL COMPOSITION OF BI-MAGNETIC CORE-SHELL $Fe_3O_4/Zn_xCo_{1-x}Fe_2O_4$ NANOPARTICLES

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We design exchange-biased magnetic nanostructures; bimagnetic core/shell nanoparticles have been fabricated by a thermal decomposition method and systematically studied as a function of the shell composition [1]. By using this nanostructure, we report a simple and effective way to control the heat generation of a magnetic colloid under alternate magnetic fields by changing the shell composition of bimagnetic core–shell Fe3O4 / ZnxCo1−xFe2O4 nanoparticles, and the effective anisotropy that can be tuned by the substitution of Co2+ by Zn2+ ions in the shell [2].
Magnetic hyperthermia experiments of nanoparticles dispersed in hexane and butter oil showed that the magnetic relaxation is dominated by Brown relaxation mechanism in samples with higher anisotropy (i.e., larger concentration of Co within the shell) yielding high specific power absorption values in low viscosity media as hexane. Increasing the Zn concentration of the shell, diminishes the magnetic anisotropy, which results in a change to a Néel relaxation that dominates the process when the nanoparticles are dispersed in a high viscosity medium. We demonstrate that tuning the Zn contents at the shell of these exchange-coupled core/shell nanoparticles provides a way to control the magnetic anisotropy without loss of saturation magnetization. This ability is an essential prerequisite for most biomedical applications, where high viscosities and capturing mechanisms are present.

[1] G.C. Lavorato, E. Lima, H.E. Troiani, R.D. Zysler, E.L. Winkler, Nanoscale 9, 10240 (2017)
[2] F.Fabris et al., Nanoscale 11, 3164 (2019)

IT9

Strongly Exchange Coupled Core|Shell Nanoparticles with High Magnetic Anisotropy: A Strategy Toward Rare-Earth-Free Permanent Magnets

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Magnetic nanoparticles (NPs) have attracted a great interest in the last decades thanks to their novel fundamental properties emerging from their extremely reduced size. Special attention has been devoted to Co-ferrite NPs due to their cheap manufacturing and high magnetic anisotropy. In particular, the application of Co-ferrite in the realization of permanent magnet has attracted a renewed interest as an alternative to rare-earth base materials in low energy applications. Therefore, a deeper understanding of the structural, size-dependent and morphological effects on final magnetic properties appears necessary. Herein, we present the chemical synthesis of a series of Co-ferrite NPs with a broad range of particle sizes (from 4 to 60 nm). We evaluated the (BH)max product, the figure of merit of permanent magnets, obtaining the maximum values ever reported in the literature for Co-ferrite NPs (i.e., 2.1 MGOe). Moreover, In a second step, we have used these Co-ferrite NPs for building blocks of more complex heterostructures based on antiferromagnetic(AFM)|ferrimagnetic(FiM) core|shell (CS) particles. The CS structure has been generated by topotaxial oxidation of the core region. The sharp interface, the high structural matching between both phases and the good crystallinity of the AFM material have been structurally demonstrated and are corroborated by the robust exchange-coupling between AFM and FiM phases. These properties induce a huge improvement of the capability of storing the energy of the material, a result which suggests that the combination of highly anisotropic AFM|FiM materials can be an effective strategy towards the realization of novel rare-earth-free permanent magnets.

IT10

SURFACE COATING EFFECTS ON THE MAGNETIC PROPERTIES OF SPINEL FERRITES NANOPARTICLES

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Since the surface plays a key role in the determining the magnetic properties of ultrasmall particles, in the last years a growing interest has been devoted to surface modification and fuctionalization by suitable coatings in order to optimize the magnetic properties for specific applications.
In this work we investigated the effect of the interaction between organic coatings and the surface of spinel ferrite nanoparticles: a) $CoFe_2O4$ particles coated with two different organic ligands (diethylene glycol: DEG) and oleic acid (OA); b) $MnFe_2O_4$ particles coated with Albumin. The investigation was carried out combining magnetization and Mossbauer spectroscopy measurements with physical modeling by DFT and Monte Carlo simulations.
The ensemble of results (1) on $CoFe_2O_4$ particles (average size: 5 nm) show a higher blocking temperature and saturation magnetization and a lower coercive field for the DEG coated particles with respect to the OA coated particles. This is attributed to the larger magnetic moments, resulting in the enhancement of dipolar interaction strength, and to the lower magnetocrystalline anisotropy of the DEG sample , as demonstrated by DFT calculations.
The ensemble of results (2) on Albumin coated $MnFe_2O_4$ particles (average size: 2 nm) show that coating produces a change in the structure, actual size and shape distribution of clusters of exchange coupled particles. Moreover, the coating produces the decrease of the magnetization and surface anisotropy, resulting in a large decrease of the coercive field. Remarkably, the coating does not affect the strength of the dipolar interactions, as shown by the same freezing temperature in the uncoated and coated particles.

1)M. Vasilakaki, N.Ntallis, N.Yaacoub, G. Muscas, D. Peddis and K.N. Trohidou, Nanoscale 10(45) 21244 (2018)
2) M. Vasilakaki, N.Ntallis, M. Bellusci, F. Varsano, R. Nathieu, D. Fiorani, D. Peddis and K.N. Trohidou, Nanotechnology 31, 025707 (2020)

IT11

Magnetic behavior of binary assemblies of nanoparticles

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We study the effect of the competition between single particle anisotropy and dipolar interactions on the magnetic behavior of binary assemblies of oxide magnetic nanoparticles with low/high anisotropy using a multi-scale modeling approach.

Models at different length scales have been used to describe our systems [1]: First an atomic scale model of a single nanoparticle that includes its size and morphology has been developed to describe the intra-particle characteristics. A mesoscopic model based on a Monte-Carlo approach is then introduced to simulate assemblies of nanoparticles by rescaling the atomic scale parameters of magnetic core/ surface nanoparticles by reducing the number of spins to be simulated to the minimum necessary to satisfactorily represent their magnetic structure. We will apply our multiscale modelling approach in two systems of binary assemblies.

First, a diluted binary ferrofluid of $MnFe_2O_4$ and $CoFe_2O_4$ nanoparticles has been investigated. The simulations of the magnetic properties are getting input from cryogenic TEM images [2] for the spatial distribution of the nanoparticles. It is shown that even at a low particle concentration, $MnFe_2O_4$ and $CoFe_2O_4$ nanoparticles interact through short distance magnetic dipole interactions within small nanoparticle clusters, which results in the sizeable reduction of the coercivity and the blocking temperature of the $CoFe_2O_4$ component and in the increase of both the coercivity and the blocking temperature of the $MnFe_2O_4$ one.

Next, we study the magnetic behavior of a dense binary assembly of γ-Fe_2O_3 and Co-doped maghemite nanoparticles [3]. We start from a pure γ-Fe_2O_3 dense assembly and we gradually substitute maghemite with Co-doped maghemite. Our study shows that the hysteresis characteristics of the binary assembly at low temperature provide evidence of the weak dipolar coupling between the two different nanoparticle populations which however it is strong enough to modify the individual hysteresis behaviour. Interestingly, the blocking temperature increases non-linearly almost two times from the corresponding pure γ-Fe_2O_3 assembly through the binary assembly to the pure Co-doped maghemite nanoparticles assembly.

In both systems are numerical results are in good agreement with experimental findings [2, 3].

[1] M. Vasilakaki, N. Ntallis, N. Yaacoub, G. Muscas, D. Peddis, K. N. Trohidou, *Nanoscale* **2018**, *10*, 21244; G. Margaris, K. N. Trohidou, J. Nogués, *Adv. Mater.* **2012**, *24*, 4331.

[2] N. Daffé, J. Zečević, M. Sikora, K. Trohidou, M. Vasilakaki, M. Rovezzi, N. Bouldi, V. Gavrilov, S. Neveu, F. Choueikani, V. Dupuis, P. Sainctavit, A. Juhin, **2019**, submitted.

[3] E. H. Sánchez, M. Vasilakaki, S. S. Lee, P. S. Normile, M. Murgia, M. S. Andersson, G. Singh, R. Mathieu, P. Nordblad, P. C. Ricci, K. N. Trohidou, J. Nogués, J. A. de Toro, **2019**, submitted.

IT12

Towards a thorough understanding of the photophysics of Carbon Nanodots - Paving the way to fully harness their potential in photo-nano-technologies

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After more than a decade from their original discovery, Carbon dots (CDs) are still attracting a large and interdisciplinary research interest in nanoscience. CDs can be described as a broad class of surface-functionalized carbonaceous nanoparticles displaying optical properties comparable to semiconductor nanocrystals, such as a bright and tunable fluorescence and marked electron donating and accepting capabilities. However, they present a series of key advantages with respect to other optical materials, such as non-toxicity, low cost, stability and ease of synthesis. Therefore, CDs are being intensely studied by many research groups committed to direct and optimize their properties to real-world applications. A serious and ongoing problem in the field of CDs is a generally limited understanding of their basic photophysics, which is crucial to fully harness their potential in nanotechnologies. In fact, several important questions remain open on the optical response of CDs, their interaction pathways with the environment or with other coupled nanomaterials, the nature of the emissive electronic transitions, and how the latter are related the underlying chemical structure, which is very synthesis-dependent.

The LaBAM group at University of Palermo has been active for a few years in the study of CDs, by combining a variety of experimental approaches and involving an extensive range of collaborations. Here we present a selection of our most recent results, addressing the photophysics of different types of CDs and CD-based nano-composites at the most fundamental level, through a range of methods capable of unraveling their photocycle from the steady-state down to sub-picosecond time scales. Thereby, we demonstrate and classify different forms of interplay between core and surface chemical moieties in CDs, and we demonstrate the key role of structural dot-to-dot disorder and small size, in determining the unique excitation/de-excitation mechanism and interactions of different types of CDs.

IT13

The carbon beyond the gold: a novel insight on the potentialities of ligand-free pulsed laser ablation of a gold target in water

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We report a novel insight in the ligand-free pulsed laser ablation (PLA) of a gold target in water. Although being a process deeply studied in the past two decades, the parallel synthesis of luminescent carbon nanomaterial has been never experimentally observed. We show in this research that the presence of NaOH as atmospheric CO$_2$ absorber in the water environment induces the simultaneous synthesis of different kind of carbon based nanomaterials. Together with carbynoid-encapsulated gold nanoparticles (Au@Cy NPs) [1], also nanotube like carbynoid nanocrystals (Au@Cy NTs) [2] and carbon quantum dots (CQDs) in both graphitic and onion-like form are found as possible multiple products of the PLA process. After a clean and simple separation process, the colloidal solution of CQDs presents an intense photoluminescence in the blue region, and we demonstrate its application as efficient optical nanoprobes for the specific sensing of methylmercury (CH_3Hg^+) ion in water. In view of biological or medical applications of the ultrasmall Au@cy NCs and CQDs, the cytotoxicity of the synthesized nanomaterial is finally investigated by optical microscopy, monitoring the uptake by different human cell lines. The results highlight an unrevealed feature of the PLA of metal target in water which has been unobserved along two decades, and offers new strategies and possibilities in the synthesis of novel biocompatible carbon based nanomaterial with unique structural, optical and functional properties.

1) T. Del Rosso, S.R.W.Louro, F.L.Deepak, E.C.Romani, Q.Zaman, Tahir, O.Pandoli, M.Cremona, F.L.Freire Junior, P.A.A.De Beule, T.De St. Pierre, R.Q.Aucelio, G.Mariotto, S.Gemini-Piperni, A.R.Ribeiro, S.M.Landi, A.Magalhães, Biocompatible Au@Carbynoid/Pluronic-F127 nanocomposites synthesized by pulsed laser ablation assisted CO$_2$ recycling, Appl. Surf. Sci., 441, pp.347-355, (2018)
2) B. Pan, J. Xiao, J. Li, P. Liu, C. Wang, G. Yang, Carbyne with finite length: the onedimensional sp carbon, Sci. Adv. 1 (2015) e1500857.

IT14

Electronic tongue: multisensor array for classification and quantitative analysis of liquid samples

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Electronic tongue (ET) is an instrument comprised by an array of non-specific and low-selectivity chemical sensors with cross-sensitivity to different species in solution and an appropriate method of pattern recognition and/or multivariate calibration for data processing. It can be employed to measure and compare tastes, as a cyber version of the mammalian gustatory system, and can also classify and quantify the chemical composition of complex liquid samples. Many examples of ET systems can be found in the literature and even commercially available. The present invited speech will cover the main aspects of ET's technology, including a brief historical overview, principles of operation, types of sensor units, and practical problems addressed nowadays. The emphasis will be given to impedimetric ET's based on sensor units made of ultrathin films of nanomaterials.

[1] M. A. Gross et al., RSC Adv. 4, 17917 (2014).
[2] L. G. Paterno, M. A. G Soler, JOM 65, 1 (2013).
[3] Yu. Vlasov et al., Pure Appl. Chem. 77, 1965 (2005).

IT15

Recent Advancements in Nano-Fluid Thermoelectric Research

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Thermoelectric technology continues to attract attention because of its potential to convert huge amounts of heat energy, which is otherwise lost, into useful electricity. The use of nanostructured solid materials (*e.g.,* texturing and porosity control, inclusions of nanoscale grains or nanoparticles within a bulk matrix etc.) has allowed tremendous improvements in the thermoelectric performance of materials as compared to that of the bulk in the last three decades. More recently, due to their extremely high Seebeck coefficients [1], certain complex liquids and their hybrid materials are also garnering increased recognition as a possible alternative to solid thermoelectrics [2]. ILs in particular, present many promising features such as high electrical conductivity, large temperature and electrochemical windows, low vapor pressure and toxicity, and raw material abundance [3]. The inclusion of charged nanoparticles has also been reported to enhance the overall Seebeck coefficient of the base-fluids [4,5]. From the application operation point-of-view, the benefit of using nanostructured electrodes has been demonstrated to increase the device performance [6].

In this presentation, I will give a review on recent findings on how nanomaterials are incorporated in the complex fluid thermoelectric research, either as a fluid additive or as device component. The current theoretical and phenomenological understanding on the multiple thermo-electro-chemical processes as well as future research and technological possibilities for thermoelectric complex fluids will be discussed.
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[1] M. Bonetti et al., "Huge Seebeck coefficients in nonaqueous electrolytes," J. Chem Phys 134, 114513 (2011).
[2] See, for example: M. F. Dupont et al., "Thermo-electrochemical cells for waste heat harvesting – progress and perspectives," ChemCom (2017), DOI: 10.1039/c7cc02160g
[3] D. R. MacFarlane et al., "Energy applications of ionic liquids," ENERGY & ENVIRONMENTAL SCIENCE, 7, 232 (2014)
[4] T. Salez et al., "Can charged colloidal particles increase the thermoelectric energy conversion efficiency?" Phys. Chem. Phys, 19, 9409 (2017).
[5] T. Salez, et al., "Magnetic enhancement of Seebeck coefficient in ferrofluids," Nanoscale Advances, 1, 2979-2989 (2019). doi: 10.1039/c9na00109c
[6] M. Bonetti et al., "Thermoelectric energy recovery at ionic-liquid/electrode interface," J. Chem. Phys. 142, 244708 (2015); doi: 10.1063/1.4923199.

IT16

CAN INFRARED SURFACE TEMPERATURE MEASUREMENTS BE USED TO DETERMINE INTRATUMORAL THERMAL DOSE DURING MAGNETIC NANOPARTICLE HYPERTHERMIA

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Non-invasive clinical thermal dose determination is traditionally obtained by the analysis of magnetic resonance data during the thermal medicine therapeutic procedure (RF ablation, HIFU, photothermal therapy, among others). This technique, however, has limited application on magnetic nanoparticle hyperthermia (MNH), since the magnetic moment of the nanoparticles is blocked inside the MRI permanent magnet, and therefore is not able to generate heat. To address this problem, we started developing a near-infrared magnetic nanocarrier that is able to be intratumorally localized by Fluorescence Molecular Tomography. The animal body reconstruction is obtained using photogrammetry, while the 3D tumor shape is determined using ultrasound. Those informations are then included in COMSOL Multiphysics and used as an input for computer simulations. Comparison between the surface temperature of the tumor monitored experimentally by thermal camera and the computer simulations, taking into account the perfusion temperature dependence and a pixel dependent heat generation function that accounts for the non-uniform particle distribution, were performed. The criteria for a good simulation were established when higher than 50% of the area under analysis (25 pixels X 30 pixels - 16mmX19mm), corresponding to 750 non-invasive thermometers, was in accordance within the temperature error associated to the experimental setup. Four animals that passed through 30-minute magnetic nanoparticle hyperthermia therapy, after intratumoral injection of the multifunctional nanocarrier, were analysed. One was sacrificed after the MNH for histopathological analysis, and served as a control. The tumor was cut in 110 slices and the total necrotic area of the treated tumor was found. Computer simulations predictions were then used to determine the critical parameter for irreversible lesion in the Ehrlich murine tumor model through the comparison with histopathological data. The other three animals were monitored up to 600 days, where one showed tumor recurrence and the other two complete regression, that correspond to a 67% survival rate. The method is then successfully applied to explain the pre-clinical observations, i.e. from the simulations we found that animals that showed complete regression had higher than 96% of irreversible lesion in the tumor, while for the animal that showed cancer recurrence we found a much lower value, 53%. The results suggest that it is possible to determine non-invasively the intratumoral thermal dose through the surface temperature monitoring during MNH if the heat centers localisation and the three-dimension tumor shape are well known.

IT17

Low-dimensional assemblies of magnetic nanoparticles improve in vitro heating power through dipolar Interactions

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Magnetic fluid hyperthermia (MFH) is a oncology clinical therapy consisting of raising the temperature of tumor cells using magnetic nanoparticles (MNPs) as heating agents. Although MFH has proven successful in treating some types of cancer, the low heating power generated under physiological conditions is the main bottleneck for making it competitive against other current cancer therapies. This low heating power makes necessary to have a high local concentration of MNPs at tumor sites, which rise toxicological question when applied in animal models.

Here, we report how the heating power of MNPs *in vitro* can be enhanced by intracellular low-dimensional clusters through a twofold strategy that includes: a) the design of the MNPs to retain Néel magnetic relaxation in high viscosity media, and b) culturing MNP-loaded cells under magnetic fields to produce elongated intracellular agglomerates. Our systematic *in vitro* experiments demonstrated that the specific loss power (SLP) of elongated agglomerates induced *in situ* by a dc magnetic field exhibited a ≈2-fold increase compared to the SLP from aggregates freely formed within cells. A numerical mean-field model that included dipolar interactions quantitatively reproduced the SLPs of these clusters both in phantoms and *in vitro*, suggesting that it captures the relevant mechanisms behind power losses under high-viscosity conditions. These results indicate that *in situ* assembling of MNPs into low-dimensional structures can help improve the heating performance in MFH.

IT18

Magnetoimmunoassays for health and healthy wine

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One of the main pillars of today's health care is prevention through immunization, good life habits, disease surveillance and screening. The last two are tightly linked to bioanalytical techniques that should, ideally, be sensitive, specific, fast and inexpensive.

These requirements are accomplished by lateral flow immunoassays (LFIA). The most popular example of LFIA is the home pregnancy test strip. Thanks to the advances in immunology, the method has been lately extended with great success to a large variety of targets as cancer biomarkers, viruses, and food contaminants [1]. To its rapidity and market low cost, LFIA adds friendly use and portability.

The key of this method is a strip of paper along which the liquid sample (urine, saliva, blood, serum or plasma) flows by capillary action, and the molecule of interest is selectively immobilized. To make it visible, the analyte is specifically labelled by colored or fluorescent nanoparticles detectable by the naked eye that provide a yes/no response.

Lately, magnetic nanoparticles are being used as LFIA alternative labels to provide a reliable and sensitive quantification [2,3]. Magnetic nanoparticles produce a magnetic perturbation that can be detected by an adequate magnetic sensor without being influenced by optical interferences [4]. Besides, magnetism can be used for pre-concentration or separation of the target analyte from the sample matrix, which can enormously help to enhance the sensitivity without complex manipulation.

This talk will review the criteria that magnetic nanoparticles need to match to be used as reporters in LFIA and how their signal can be read out to provide a useful analytical tool for biomedicine and food safety applications.

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[1] R. Wong, H. Tse. "Lateral flow immunoassay", Humana Press; New York, NY, USA: 2009
[2] Y. Wang, H. Xu, M. Wei, H. Gu, Q. Xu, W. Zhu, Mat. Sci. Eng.: C, 29 (3), 714 (2009).
[3] A. Moyano, M. Salvador, J.C. Martínez-García, V. Socoliuc, L. Vékás, D. Peddis, et al., Anal Bioanal Chem 411 (25), 6615 (2019)
[4] D. Lago-Cachón, M. Oliveira-Rodríguez, M. Rivas, M.C. Blanco-López, J.C. Martínez-García, A. Moyano, et al, IEEE Magn. Lett. 8, 1 (2017).

IT19

Detailed Structural Characterization of Nanomaterials by Precession Electron Diffraction

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Transmission electron microscopy TEM) is usually applied to analyze nanosystems with structural and spectroscopic methods with nanometric and atomic resolution. When the electron travels across the sample, the strong electron-matter interaction generates multiple scattering events even when we deal with very thin few nm samples sample. This physical phenomenon is called “dynamical diffraction” and makes rather difficult the difficult the understanding and modelling of diffracted beam intensities or image contrast in atomic resolution pictures. In recent years the use of precession electron diffraction (PED) has been shown to provide an excellent approach to overcome up to certain degree this complex electron diffraction issue. In fact, the contribution of dynamical scattering can be significantly reduced and diffracted intensities can be described as “quase-kinematical”, where simpler methods -usually associated with X-ray- become applicable. The residues of several crystallographic techniques can be significantly reduced by associating electron diffraction with precession, as for example in Pair Distribution Function (PDF) approaches. When PED is acquired with a scanning nanometric electron beam (spatially resolved PED), we can map structural properties and even subtle deformations fields in individual nanostructures. We will discuss different application examples to nanoparticles and nanowires that clearly show the high relevance of the PED approach for the fine characterization of nanoscale materials.

IT20

Decreasing Nanocrystal Structural Disorder by Ligand Exchange: An Experimental and Theoretical Analysis

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Nanocrystals (NCs) present unique physicochemical properties arising from their size and the presence of ligands. Comprehending and controlling the ligand−crystal interactions as well as the ligand exchange process is one of the central themes in NC science nowadays. However, the relationship between NC structural disorder and the ligand exchange effect in the NC atomic structure is not yet sufficiently understood. Here we combine pair distribution function analysis from electron diffraction data, extended X ray absorption fine structure, and high-resolution transmission electron microscopy as experimental techniques and first-principles density functional theory calculations to elucidate the ligand exchange effects in the ZrO_2 NC structure. We report a substantial decrease in the structural disorder for ZrO_2 NCs caused by strain rearrangements during the ligand exchange process. These results can have a direct impact on the development of functional nanomaterials, especially in properties controlled by structural disorder [1].

[1] G. R. Schleder et al., J. Phys. Chem. Lett. 2019, 10, 1471−1476

IT21

Ferrofluids in ionic liquids: high temperature study

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Ferrofluids in ionic liquids are interesting fluids which combine magnetic properties with the advantages of ionic liquids, a broad class of liquids, that consist solely of ions, and can be liquid at room temperature, presenting interesting properties as a low vapor pressure, a large electrochemical window, and possible stability at high temperatures. The dispersion of nanoparticles (NPs), here magnetic maghemites of diameter around 8 nm, in an ionic liquid is however not obvious as the usual approaches for colloids in molecular solvent cannot be applied. Our studies at room temperature in EAN [1] and more recently in many other ionic liquids [2] have shown the ability to disperse charged NPs in ILs at room temperature controlling the solid/liquid interface, i.e. the charge of the surface, the groups producing this charge and the initial counterions of the nanoparticles. The interparticle interactions can vary from weakly repulsive to weakly attractive depending on the precise composition of the systems and long term stable colloidal dispersions can be obtained. We explore here these systems at high temperature up to 200°C, and determine the nanostructure and interparticle interaction from a coupling of Small Angle Neutron Scattering (SANS) and Dynamic Light Scattering (DLS).

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References:

[1] M. J. Siriex-Plénet, F. Cousin, E. Dubois, V. Peyre, Soft Matter 10, 1097 (2014)
[2] J. Riedl, A. Akhavan Kazemi, F. Cousin, E. Dubois, S. Fantini, S. Loïs, R. Perzynski, and V. Peyre, submitted to Nanoscale Advances. On chemrxiv, doi:10.26434/chemrxiv.9817208.

IT22

Colloidal materials in ionic liquids: influence of ionic and water content on dispersions stability

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Dispersing nanoparticles (NP) in ionic liquids (ILs) leads to new materials with many potential applications, e.g., in catalysis or electrochemistry [1]. Usually, the material must behave as a liquid with well dispersed particles. The mechanisms driving colloidal stability in ILs require a better understanding: if the formation of protective solvent layers around the particles is now an accepted fact, their exact organization, the principles inducing this organization and the resulting interparticular forces are still under debate [2]. In former works, we showed that the nature of the NP-IL interface is of the highest importance for colloidal stability [3,4] and that a fine tuning of this interface is mandatory.

We investigate by a multiscale approach involving visual observation, dynamic light scattering, optical microscopy and small angle scattering, how the solutes present in ethylammonium nitrate (EAN) can condense on the maghemite NP surface inducing an efficient organization of the surface layer. We focus on the specific role of water, a cosolvent unavoidably present and on the addition of Na^+, Rb^+ and Li^+ as NP's counterions, since there are in competition with the cations of the IL. We propose a model for the molecular-scale organization of the layer, based on H-bond when water in present and on the size matching of ions with surface charge.

[1] He, Z., Alexandridis, P., *Adv. Coll. Interf. Sci.* **244** (2017) 54
[2] Gebbie M.A. et al, *Chem. Comm.*, **53** (2017) 1214
[3] Mamusa, M. et al., *Soft Matter* **10** (2014) 1097
[4] Guibert, C. et al, *J ; Coll. Interf. Sci.,* **454** (2015) 105

IT23

Dynamics of highly anisotropic magnetic chains

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Highly anisotropic magnetic chains may present slow magnetic relaxation and hysteresis below a blocking temperature T_b usually around or above liquid helium. They have been named “Single Chain Magnets” and many efforts have been devoted to their development since its discovery [1] due to the possibility of using as molecular magnetic memory units. In this presentation we will review the progress that has been achieved in their development and in particular the control of the magnetic relaxation by irradiation using visible light on ferrimagnetic cobalt(II) chains containing suitable polyaromatic nitronyl nitroxide radicals [2]. Results using Rare Earth ions in similar chains will also be discussed.

[1] A. Caneschi et al., Angew. Chem. Int. Ed. **40,** (2001)
[2] Maria G. F. Vaz et al., Chem. Eur. J. **20**, 5460 (2014)

IT24

DISCERNING BULK FROM INTERFACE INTERACTIONS IN MAGNETIC NANOSTRUCTURES

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During the last decades, the studies on dipolar and exchange interactions in assemblies of magnetic nanoparticles and in thin magnetic films have mostly been performed through remanence magnetization plots, e.g., δM plots. It is important to emphasize that this technique can only be applied to systems with symmetric major hysteresis loops. For such systems, a relation associating in-field magnetization (and not remanence) curves has been derived [1] in 2018, leading to an introduction of a novel, δM_R plot, which presents important advantages over the remanence one. E.g., δM_R is acquired in an easier and faster manner and does not demand demagnetization so it can be applied on systems with rectangular symmetric major loops.

Recently, a general δM_R plot has been proposed [2] allowing to assess interactions even in ferromagnet/antiferromagnet (FM/AF) exchange-biased (EB) systems with asymmetric and shifted major loops. A recoil loop and the position of the center of the respective major loop are only needed for the construction of such a general δM_R plot. An asymmetric EB major loop has one of its branches steeper than the other. This leads [2] to (i) a nonzero δM_R plot obtained from the major loop, which is a footprint of the FM/AF interface coupling, and (ii) two distinct δM_R plots obtained from recoil curves, each starting from the coercive field of the descending branch of the major loop and traced for magnetic field either parallel or antiparallel to the EB direction. The analysis of these plots allows discriminating the effects coming from magnetic coupling into the bulk of the FM from those emerging at the FM/AF interface. Our model simulations indicate that, for symmetric major loops, the effects of the interface FM/AF exchange coupling might not be identified by either of the in-field magnetization plots; this interaction is only evidenced through the shift along the field axis and an enhancement of the coercivity. Applications of the method on EB thin films and core/shell nanoparticles are presented.

This work has been financed by CNPq (grants 305796/2016-0 and 422740/2018-7) and CAPES. Free software which generates δM_R plots is available [3].

[1] J. Geshev, J. Magn. Magn. Mater. 476, 135 (2018)
[2] J. Geshev *et al*., https://arxiv.org/abs/1906.04124
[3] http://www.if.ufrgs.br/pes/lam/dMr.html

IT25

The Kubo Fluctuation-Dissipation Theorem

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In this short talk we revisit the fluctuation-dissipation theorem [1] and recent developments in its generalization to nonequilibrium systems [2]. Within the framework, we discuss linear response and Onsager's relation along with power dissipated by external work performed on exemplary systems. Applications of the FDT in the study of fundamental properties of certain processes, mainly in condensed matter physics, chemistry and biology will be emphasized. Concepts of the generalized FDT in the analysis and characterization of various diffusive regimes will be addressed and its links with the memory function will be provided, showing limits of the applicability of the theorem [3] and the hierarchy connecting irreversibility, ergodicity and FDT [4,5].

[1] R. Kubo Prog Phys. (1966) 29:255. doi: 10.1088/0034-4885/29/1/306.
[2] U. M. B. Marconi et al., Phys. Report 461, 111 (2008)
[3] I. V. L. Costa, R. Morgado, M.V.B.T. Lima, EPL 63, 173 (2003).
[4] L. C. Lapas, R. Morgado, M. H. Vainstein, J. M. Rub__, and F. A. Oliveira, Phys. Rev. Lett. 101, 230602 (2008).
[5] F. A. Oliveira, R. M. S. Ferreira, L. C. Lapas, and M. H. Vainstein, Review, Frontiers in Physics 7 18 (2019) (https://doi.org/10.3389/fphy.2019.00018)

IT26

FROM SYNTHESIS TO APPLICATIONS: DESIGN OF NANOMATERIALS FOR PROPERTY CONTROL

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In the field of applied research, offering innovative materials with new properties is an ever-present challenge. These properties are specific to each application. In order to get close to it, the four main characteristics of a material must be perfectly mastered. The first, which governs its intrinsic properties, is its composition and the crystalline phase obtained in the case of crystalline solids.

The second is the size of the primary objects that make up the solid. On a larger scale, texturing (porous materials, multi-scale architectures, superstructures...) is also used. Finally, the shaping of materials (films, powders...) is the last of these four characteristics that dictate the properties of the material within the final device. On the fundamental research side, it is essential to understand the relationship between structure/morphology/texture and targeted property. Indeed, the synthesis of the material must not be done in a "trial and error" approach but on the contrary it must be at the heart of a real understanding of the parameters governing reactivity.

Despite the abundance of crystalline phases associated with metals, oxides, carbides... new structures are regularly discovered and often possess original properties. Indeed, often inaccessible by the traditional synthesis methods, they have proved to be effective thanks to softer and more innovative synthesis methods such as Sol-Gel chemistry. This synthesis pathway, which operates at low temperature, makes it possible to reach metastable states of matter by often favoring kinetic control over thermodynamic control. In addition, some phases exist only for extremely small particle sizes corresponding to the nanoscale. The control of Sol-Gel chemistry and its determining parameters (typically concentration, temperature or pH in the case of aqueous solutions) is the most suitable way to structure the material on this scale.

We will see some examples of nanooxides (TiO_2, WO_3…) for Energy and Environment.

IT27

AMORPHOUS, PARTIALLY CRYSTALLINE AND CRYSTALLINE MAGNETIC MICROWIRES: FROM FABRICATION AND PROPERTIES TO PRACTICAL APPLICATIONS

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A family of ferromagnetic wires is very big. It consists of wires with different dimensions and shapes. In this work we considered three types of glass-coated microwires with cylindrical symmetry: i) Co-, Fe- and CoFe-based amorphous ferromagnetic microwires [1]; ii) partially crystalline Co-, Fe- and CoFe-based microwires [2]; iii) fully crystalline Heusler alloy-based microwires [3]. Single microwires or microwires-based arrays can be used in Security control system – as magnetic tags, in Coding systems, as Universal ultrasensitive sensors of magnetic fields, mechanical stresses, temperatures, deformation and other physical parameters, Energy saving machines, Induction systems in microelectronics, as Basic part for lossy jacket, in Medical applications (prosthetic device, tweezers, sensors etc.).

TEM, SEM, XRD analysis were used to study the structural properties. Magnetic field dependence of the velocity of the domain wall propagation was measured by Sixtus-Tonks method, the hysteresis loops – by induction or vibrating sample magnetometry methods and both the local nucleation fields distribution and magnetostriction coefficient – using special custom devices. Magnetic interactions were analyzed using FORC analysis. Competition between the magnetostatic and magnetoelastic coupling leads to possibility to vary the magnetization mechanisms and, as a results a number and value of the switching fields. This tuning can be widely use for applications. In additional, the size effect on the magnetization process is considered and analyzed.

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[1] I. Baraban, S. Leble, L.V. Panina, V. Rodionova, Journal of Magnetism and Magnetic Materials, 477 (2019) 415-419, https://doi.org/10.1016/j.jmmm.2018.12.017;
[2] Rodionova V.V., Baraban I.A., Panina L.V., Bazlov A.I., and Perov N.S., IEEE Transactions on Magnetics (1.467), 54 (11) (2018), DOI: 10.1109/TMAG.2018.2855977;
[3] S. Shevyrtalov, A. Zhukov, I. Lyatun, S. Medvedeva, H. Miki, V. Zhukova, V. Rodionova, Journal of Alloys and Compounds (3.779), 745 (2018) 217–221, https://doi.org/10.1016/j.jallcom.2018.02.096.

IT28

Design advanced magnetic nanocomposites based on transition metal oxides

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Magnetic nanocomposites (MN) represent an important class of technologically relevant materials, in particular for several applications ranging from biomedicine, catalysis, and energy devices. The properties of magnetic nanocomposites rely strongly on the interplay between those of the constituent components. When the individual components themselves, are complex systems belonging to the family of correlated electron oxide wuth exotic physical properties[1], it becomes non-trivial to customize the properties of the nanocomposite. In this work, we will discuss the design of advanced magnetic nanocomposites based on transition metal oxides, focusing on key factors influencing magnetic properties of the material.

In order to show the effect of spatial arrangement of magnetic phase(i.e. morphology) on the magnetic properties two MN $La_{0.67}Ca_{0.33}MnO_3/CoFe_2O_4$ in similar volume fractions however arranged with different morphologies, will be presented. This morphology–physical property relationship, and the possibility to further tune the magnetism and magneto-transport in such nanocomposites will be discussed[1]. Then, It will be discussed how the magnetic coupling in bi-magnetic nanocomposites can be controlled by the growth technique. Using four different synthesis strategies to prepare prototypical $LaFeO_3$–$CoFe_2O_4$ and $LaFeO_3$–$Co_{0.5}Zn_{0.5}Fe_2O_4$ nanocomposite systems, and by performing comprehensive magnetic measurements, it will be demonstarted that the final material exhibits striking differences in their magnetic coupling that is distinct to the growth method. Through structural and morphological studies, we confirm the link between the magnetic coupling and growth methods due to distinct levels of particle agglomeration at the very microscopic scale[2]. Finally, it will be novel synthesis method by which the two components of the nanocomposite can be directly integrated with each other, yielding homogeneous samples on the nanoscale with magnetic behavior reminiscent of a single phase. We illustrate our method using multiferroic $BiFeO_3$ (BFO) and $LaFeO_3$ (LFO) as the major phase (i.e., matrix), and MFe_2O_4 ($M = Co^{2+}$ or Ni^{2+}) as the embedded magnetic phase. Furthermore, we show that by a proper selection of the second phase in the nanocomposite, it is possible to customize the magnetic properties of the matrix[3].

(1) Muscas, G.; Kumara, P. A.; Barucca, G.; Concas, G.; Varvaro, G.; Mathieu, R.; Peddis, D. Designing New Ferrite/Manganite Nanocomposites. *Nanoscale* **2016**, *8* (4), 2081–2089.
(2) Sarkar, T.; Muscas, G.; Barucca, G.; Locardi, F.; Varvaro, G.; Peddis, D.; Mathieu, R. Tunable Single-Phase Magnetic Behavior in Chemically Synthesized $AFeO_3$ -MFe_2O_4 (A = Bi or La, M = Co or Ni) Nanocomposites. *Nanoscale* **2018**, 22990–23000. https://doi.org/10.1039/C8NR06922K.
(3) Sayed, F.; Muscas, G.; Jovanovic, S.; Barucca, G.; Locardi, F.; Varvaro, G.; Peddis, D.; Mathieu, R.; Sarkar, T. Controlling Magnetic Coupling in Bi-Magnetic Nanocomposites. *Nanoscale* **2019**, *11*, 14256–14265. https://doi.org/10.1039/c9nr05364f.

IT29

DYNAMICS OF FLEXIBLE FERROMAGNETIC FILAMENTS

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Flexible ferromagnetic filaments have interesting dynamic properties. If the field polarity changes the filament buckles and makes a loop, which further relaxes through the third dimension. During this process its topological characteristics (writhe number) change. The buckling instability of the ferromagnetic filaments enables the creation of self-propelling magnetic microdevices [1]. In an AC magnetic field of enough high frequency the ferromagnetic filament orients perpendicularly to the field. Field induced bending of ferromagnetic filament contributes to magnetic susceptibility of their suspension. Solution of the corresponding boundary problem of the magnetoelasticity shows that both real and imaginary parts of magnetic susceptibility at large frequencies obey the characteristic power law $\omega^{-3/4}$. It is known that a rigide dipole in a rotating field has coexisting fixed points (centers) and periodic trajectories. This situation is structurally unstable – a small perturbation, for example a constant field along the angular velocity of the rotating field, changes the situation and fixed points become stable focuses and the precessional motion of the dipole occurs. It is illustrated numerically that flexible ferromagnetic filament behaves similarly – at frequencies above the critical it carries out synchronously with the field precessional motion around its angular velocity .This result is confirmed experimentally [2].

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[1]. A.Cēbers, and K.Ērglis. Adv.Func.Mat., 26,3783 (2016)
[2]. A.Zaben, G.Kitenbergs, and A.Cēbers. arXiv:1908.02604 (2019)

IT30

DUAL REVERSAL MODES BY HELICITY CONTROL IN FERROMAGNETIC NANOTUBES: MONTE CARLO SIMULATION AND MICROMAGNETIC APPROACH

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In this work, the low-temperature magnetic configurations, summarized in phase diagrams, as well as the magnetization reversal modes of ferromagnetic nanotubes, are investigated. Results were conducted by using standard Metropolis Monte Carlo simulations of single-wall zig-zag ferromagnetic nanotubes of different aspect ratios and by using also micromagnetic calculations for FeCo nanotubes. Classical Heisenberg magnetic moments interacting via competing short-range exchange (J) and long-range dipolar interactions (of strength D) were considered. Results reveal the occurrence of different low-temperature magnetic states depending of the degree of competition between the exchange and dipolar energies. Thus, collinear ferromagnetic (FM) states are observed for dominant exchange interactions whereas helical (H) and subsequent vortex (V) states are obtained above a certain threshold value of $\gamma=D/J$ when dipolar interactions become relevant. By using suitable order parameters, we propose a series of magnetic phase diagrams as a function of γ, radius (N) and height (N_z) of the nanotubes [1]. The occurrence of transient circular states during magnetization reversal, when a uniform external field is applied parallel to the tube axis, is also influenced by the strength of dipolar interaction and aspect ratios in tubes of some few nanometers studied via Monte Carlo. Analogously, micromagnetic simulations of FeCo nanotubes of tens of nanometers with aspect ratios similar to those studied by Monte Carlo, reveal also the presence of such states. Moreover, two different magnetization switching modes are feasible. One (Q_1), characterized by intermediate stages having H states at the ends of the tube with the same chirality with a low-coercive field. A second one (Q_2) with opposite chiralities and a high-coercive field, where regions magnetically harder in the middle of the tube during inversion appear as a consequence of a merging process of the circular states. Energy calculations suggest that both modes are interconnected in the energy landscape. Our results can shed lights on a new mechanism for coercivity enhancement, and for understanding the hysteretic properties of tubular nanostructures where dipolar interactions play a key role.

[1] H. D. Salinas, J. Restrepo, Òscar Iglesias, *Sci. Rep.* **8** (2018) 10275.

IT31

Alginate@PLGA nanocomposite beads for the prolonged delivery of haloperidol antipsychotic to the brain via an oral route

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Currently therapeutic treatments for schizophrenia, intravenously or orally, are only partially effective and generally associated with extrapyramidal effects often dangerous and very troublesome for patients. In order to increase the treatment efficiency while limiting any side effects, the aim of this work was to design composite capsules (PLGA-PEG/alginate) intended to be administered by an oral route and able to release locally, in a specific and controlled way, the neuroleptic “haloperidol” in the brain. The optimization of the protocol of synthesis allowed to obtain in a reproductible way, porous PLGA nanoparticles, having an average hydrodynamic diameter between 60 to 250 nm and a good stability in aqueous solution. Once functionalized with PEG-diamine, in vitro studies showed the low toxicity of these nanoparticles as well as their ability to encapsulate a satisfactory amount of haloperidol and release this active principle over a period of one month with low burst effect. The incorporation of PEGylated nanoparticles in matrices prepared with a high concentration of alginate made it possible to obtain nanocomposite beads having a good stability at the exit from the simulated gastric medium and persisting approximately 30 minutes in simulated intestinal medium. Finally, preliminary studies in vivo on adult mice using injected nanoparticles and ingested nanocomposite beads showed the effectiveness of these system to deliver haloperidol in the brain.

IT32

Application of core@shell based magnetic nanoadsorbents for water remediation

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The magnetic separation technology using nanoadsorbents has been emerging as a promising strategy to remove pollutants from water easily and economically [1]. Indeed, the spatial confinement of the adsorbent to the nanoscale together with the possibility of magnetic manipulation endow the material with unique properties such as large surface area and magnetic retrieval, allowing fast pollutant removal and possibility of recovery and reuse. In this context, the present survey focuses on the elaboration, characterization and application of magnetic nanoadsorbents based on core-shell nanoparticles for removal of different types of pollutants (toxic metals, dyes, BTEX and pharmaceuticals) from water [2-4]. These nanoadsorbents combine several constituent materials and properties in a single object. Their suitability is investigated as a function of mean size in different controlled conditions of pH, shaking rate, initial pollutant concentration, contact time and temperature. The competitive influence of representative interferents in the adsorption efficiency is checked individually and in synthetic wastewater. Moreover, the regeneration capacity and reusability of the nanoadsorbents is examined. The results serve as a basis for applying the proposed magnetic nanoadsorbents in large-scale setups to test their performance in real polluted samples.

[1] D. Mehta, S. Mazumdar, S.K. Singh, J. Water Process. Eng. 7, 244 (2015)
[2] F. L. Rodovalho, G. Capistrano, J. A. Gomes, F. F. Sodré, J. A. Chaker, A. F. C. Campos, A. F. Bakuzis, M. H. Sousa, Chem. Eng. J. 302, 725 (2016)
[3] A. F. C. Campos, H. A. L. de Oliveira, F. N. da Silva, F. G. da Silva, P. Coppola, R. Aquino, A. Mezzi, J. Depeyrot, J. Hazard. Mater. 362, 82 (2019)
[4] A. F. C. Campos, P. H. Michels-Brito, F. G. da Silva, R. C. Gomes, G. Gomide, J. Depeyrot Journal of Environmental Chemical Engineering 7, 103031 (2019)

ORAL PRESENTATION

OC1

MULTIFERROIC POLYMER COMPOSITE BASED ON HEUSLER-TYPE MAGNETIC MICROWIRES WITH COMBINED MAGNETOCALORIC AND MAGNETOELECTRIC EFFECTS

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Recently, the great scientific interest has focused on the design of smart materials, which exhibit large caloric effects (CE) combined with strong magnetoelectric (ME) coupling, for biomedicine and energy efficient technologies. As it is known, multiferroics are materials which demonstrate the coexistence of at least two ferro ordering (magnetic, electric, mechanical) and hence they were proposed as candidates for multicaloric materials. Magnetoelectric (ME) composites consisted of piezoelectric and magnetic phase can exhibit «giant» ME response trough mechanical interactions between components due to the magnetostrictive and piezoelectric effects. Thus, the multiferroic composites were suggested as candidates for multicalorics and the ME effect –for enhance and control of the caloric effects. Recently a search for multicalorics with large caloric effects and magnetoelectric coupling around room temperature is attracted considerable attention [1, 2].

We studied the magnetocaloric and magnetoelectric properties of the new type of ME composite consisted of Heusler-type magnetic microwires embedded in polyvinylidene fluoride polymer matrix fabricated using modified solvent casting technique. The maximum in adiabatic temperature change ΔT about ~0.04 K were observed around 276 K with narrow hysteresis accompanied with maximum of magnetoelectric coefficient. Observed temperature dependences of magnetocaloric and magentoelectric effects could be associated with both magnetic (paramagnetic-ferromagnetic) and structural (austenite-martensite) phase transitions. The measurements of magnetocaloric effect in modes with different frequencies of modulated magnetic field exhibit the reduction of ΔT about 38 % with increase of frequency from 0.5 Hz to 20 Hz.

[1] Ce-Wen Nan, M. I. Bichurin, Shuxiang Dong, D. Viehland, and G. Srinivasan, Multiferroic magnetoelectric composites: Historical perspective, status, and future directions, J. Appl. Phys. 103 (2008) 031101;
[2] I. A. Starkov, A. Starkov, A generalized thermodynamic theory of the multicaloric effect in single-phase solids, International Journal of Solids and Structures 100-101 (2016) 187-194.

OC2

GALLIUM PHOSPHIDE NANOWIRES: EPITAXIAL GROWTH AND OPTICAL PROPERTIES

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In the last years, special attention has been dedicated to obtain or control Wurtzite (WZ) crystal structure in GaP nanowires (GaP NWs) due to the conversion into a direct band gap material in the green spectral range [1-3]. Here, we have grown Au catalyzed Gallium Phosphide nanowires by chemical beam epitaxy. We show that the Au nanoparticles may become unstable, crawling in the [110] direction, depending on the growth conditions. We present several indications of how this phenomenon impacts nanowire morphology, which we interpret as leading to the formation of an WZ asymmetric nanostructure [4]. Secondly, we present a variety of optical data in order to elucidate the exact value of the fundamental band gap, excitonic emission and valence band splitting energies of the WZ phase. Our data indicates the existence of an optical band gap at low temperature at 2.20 eV as well as a pseudo-direct band gap behavior. Furthermore, we present and discuss how to control the incorporation of unintentional impurities on the luminescence by growth conditions. Finally, we show possible alternative catalysts for the growth of Gallium Phosphide and Gallium Arsenide nanowires, specially nickel (Ni) and Tin (Sn). However, the growth dynamics in this case presents a dramatic change, leading to nanostructures with very different characteristics from the gold counterpart, such as [112]-oriented nanowires. This unusual growth direction can be achieved in a controlled way, by changing the nature of the catalyst. Furthermore, high aspect ratio nanowires can be grown without the use of in-situ HCl in our CBE system.

[1] S. Assali et al., J. App. Phys.,120, (2016).
[2] De, A. and Pryor, C. E., Phys. Rev. B, 81, (2010).
[3] N. N. Halder et al., App. Phys. Lett., 112, (2018).
[4] Da Silva, B. C. et al., Nano Lett., 17, (2017).

OC3

Synthesis and characterization of GO-H_3BO_3 composite for single sensor impedimetric olfaction.

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With the goal of development of olfactive system for non-invasive clinical analysis thorough human breath olfaction, the present study shows the synthesis and characterization of graphene oxide/boric acid composite (GO-HBO) for utilization in single electrode olfaction in high humid environments. The characterization of the composite GO-HBO and bare GO was carried using scanning electronic microscopy (SEM), impedance spectroscopy (IS), structural analysis (XRD, Raman) and elementary analysis (XPS, TG). The determination of the electronic signatures of the water and aqueous solutions of ethanol or acetone, in the range of 80 to 640 ppm, was demonstrated using a single sensor interrogated with a multi-frequency signal probe regime inside a head-space system. This study contributes to the cheapening and simplification of the necessary instrumentation for electronic e-noses toward the diagnostics of diseases by analysis of human breath vapors.

[1] DA SILVA, Mauro J. **Calorim.**, v. 107, n. 1, p. 257-263, 2012.
[2] CAVALLARI, Marco R. et al. **IEEE Sens. J,**, v. 17, n. 7, p. 1971-1980, 2017.

OC4

TRANSIENT DECAY OF PHOTOINDUCED CURRENT IN THE HETEROSTRUCTURE GaAs/SnO$_2$ WITH NANOSTRUCTURED SEMICONDUCTOR OXIDE TOP LAYER

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Lattice relaxation around defects originate the phenomenon known as persistent photoconductivity (PPC), where metastably induced carriers remain in a conductive state for low enough temperature to avoid the re-trapping back. Although this hypothesis is widely accepted to explain PPC, there are other causes such as separation of excited carriers by local-potential fluctuations. In the case of nanostructured materials, the charge stored at grain boundary and the electron scattering in this region lead to additional contributions. In this work, the decay of photoinduced conductivity is measured for GaAs/SnO$_2$ heterostructure, after illumination with below (450 nm) and above (325 nm) bandgap energy of the top SnO$_2$ layer. Eu^{3+}-doped SnO$_2$ is deposited by dip-coating (crystallite size about 10nm), and the GaAs bottom layer by resistive evaporation. Decay shows unusual behavior since it gets slower as the temperature is raised. The trapping by intrabandgap defects (mainly Eu^{3+} centers and oxygen vacancies) in the SnO$_2$ layer is expected [1], but a GaAs/SnO$_2$ interface arrest becomes also evident, mainly below 100 K. A permanent variation on resistivity is observed at 50K (PPC). The 450 nm source leads to an increased permanent portion on the resistivity variation as the temperature decreases, whereas the 325 nm excitation leads to a practically constant value as the temperature decreases, which is a good indication that intrabandgap states, predominantly excited by the below bandgap light, have thermally activated cross section typical of large lattice relaxation defects. This behavior contributes for the understanding of the electrical transport in this nanostructured hybrid device which, combined with emission from Eu^{3+} ions [2], opens new possibilities for optoelectronic devices because samples in the form of films are desirable for circuit integration.

[1] C. F. Bueno, L.V.A. Scalvi, Thin Solid Films 612, 303 (2016)
[2] C. F. Bueno et. al. Opt. Mater. Express 5, 59 (2015)

OC5

Nanoscale Investigation on the Stability of Carbon Nanodots Aqueous Dispersions

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Carbon nanodots (CDs) 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, low toxicity [1]. In this study, we investigate nitrogen-enriched carbon nanodots (N-CDs) synthesized by thermally induced decomposition of organic precursors [2]. Their size and structure were checked by combined analysis of transmission electron microscopy (TEM), x-ray diffraction (XRD) and fourier-transform infrared spectroscopy (FTIR). The nanodots were dispersed in different aqueous solutions from pH 2.0 to 12.0, acidified by HNO_3 and alkalinized by NaOH at controlled ionic strength by the addition of $NaNO_3$ as a background electrolyte. Different amounts of precipitate could be observed at the macroscopical scale, which is qualitatively related to the increase in stability as the pH rises. Zeta potential measurements performed at the various pH conditions reveals an increase of the negative surface charge as the medium becomes more alkaline, in agreement with the deprotonation of carboxyl surface groups [3]. In this sense, the observed improvement in stability correlates with the increase in electrostatic repulsion between nanodots induced by the surface charge development. In order to further understand the dispersion stability properties, small angle x-ray scattering (SAXS) was performed to probe the nanodots structuralization at the nanoscale. Time dependent measurements were performed in order to probe sedimentation processes and centrifugation procedures were implemented in order to remove aggregates. The data indicates the pH has a substantial impact at the local ordering of the nanodots, providing a nanoscale insight of the instability effects observed at the macroscale. These novel results shed light on the nanoscale ordering of N-CDs as a function of the pH in aqueous dispersions allowing a deeper understanding on the colloidal stability.

[1] A. Sciortino et al., J. Phys. Chem. Letters, 7, p. 3419 (2016)
[2] L. Sciortino et al., J. Phys. Chem. C, vol. 122, no. 34, p. 19897 (2018).
[3] T. Fiuza et al., C - J. Carbon Res., vol. 5, no. 4, p. 74 (2019).

OC6

Water vapor diffusive transport in a smectite clay: Cationic control of normal versus anomalous diffusion

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The transport of chemical species in porous media is ubiquitous in subsurface processes, including contaminant transport, soil drying, and soil remediation. We study vapor transport in a multiscale porosity material, a smectite clay, in which water molecules travel in mesopores and macropores between the clay grains but can also intercalate inside the nanoporous grains, making them swell. The intercalation dynamics is known to be controlled by the type of cation that is present in the nanopores; in this case exchanging the cations from Na^+ to Li^+ accelerates the dynamics. By inferring spatial profiles of mesoporous humidity from a space-resolved measurement of grain swelling, and analyzing them with a fractional diffusion equation, we show that exchanging the cations changes mesoporous transport from Fickian to markedly subdiffusive. This results both from modifying the exchange dynamics between the mesoporous and nanoporous phases, and from the feedback of transport on the medium's permeability due to grain swelling. An important practical implication is a large difference in the time needed for vapor to permeate a given length of the clay depending on the type of intercalated cation [1].

1. Michels L., Méheust Y, Altoé M.A.S., dos Santos E.C., Hemmen H., Droppa Jr. R., Fossum J.O., da Silva G.J. **(2019)** Phys. Rev E 99, 013102

OC7

PREPARATION OF HYBRID PVDF-COFE$_2$O$_4$ SELF-STANDING FILMS FOR MAGNETOELECTRIC APPLICATIONS: IS THERE A SUSTAINABLE ALTERNATIVE TO THE USE OF DIMETHYLFORMAMIDE?

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Multiferroic materials have potential for many applications such as actuators sensors or memory devices, thanks to their magnetoelectric effect (ME). Such effect was first observed in inorganic single crystals but due to their low Curie temperature and their weak ME coupling coefficient, they were seldom integrated in devices. To overcome these limitations, the composite material strategy offers the opportunity to tune ferromagnetic and ferroelectric properties of the two phases acting on the hybrid interface. In this context, we developed new flexible multiferroic composite materials through (i) a smart tailoring of the hybrid interface between a ferroelectric and piezoelectric fluoropolymer, PVDF, crystallized in its β-polymorph, and inorganic ferrimagnetic and magnetostrictive nanoparticles (NPs), cobalt ferrite ($CoFe_2O_4$), and (ii) an effective control of NPs size [1] and surface chemistry [2].

To the best of our knowledge, up to now, there is no paper dealing with the sustainable preparation of hybrid $CoFe_2O_4$-PVDF films for magnetoelectric applications: DMF is still the most used solvent to prepare these materials since it is considered as the best solvent to induce the crystallization of PVDF in its β-polymorph. However, it is now well-known that solvents with high polarity tend to induce the crystallization of β-PVDF [3] Hence, the question raised is now: new solvents are doubtless required to improve the sustainability of the synthesis of PVDF-based films but will they be as efficient as DMF to induce the crystallization of β-PVDF in presence of 13 nm $CoFe_2O_4$ nanoparticles?

We present here our first studies on the synthesis of $CoFe_2O_4$-PVDF magnetoelectric thin films using less toxic solvents.

[1] M. Bibani, R. Breitwieser, A. Aubert, V. Loyau, S. Mercone, S. Ammar, F. Mammeri, Beilstein J Nanotechnol. 10, 1166 (2019).
[2] C. Ben Osman, E. Barthas, P. Decorse, F. Mammeri, Colloids Surface A, 577, 405 (2019).
[3] F. Mammeri, Frontiers of Nanoscience 14, 67 (2019).

OC8

INTERPARTICLE INTERACTIONS AND MAGNETIC BLOCKING PROPERTIES OF FINE FERRITE NANOPARTICLES

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Using low field DC magnetization, AC susceptibility, isothermal remanent magnetization and DC demagnetization techniques, we compare the magnetic blocking properties and remanence curves of dilute ferrofluid and powder samples based on ferrite magnetic nanoparticles, in order to investigate the role of interparticle magnetic interactions on the superparamagnetic relaxation, the magnetic anisotropy and on the super-spin-glass state in closely packed particles. Cobalt ferrite-based nanoparticles are used as sample, obtained as aqueous colloidal dispersions following a coprecipitation strategy, yielding very small core-shell particles. These samples show large anisotropy attributed to an enhanced surface contribution, blocking temperature that shifts towards higher values as interparticle distance decreases and a frequency dependency of its peak temperature being well accounted by a Vogel–Fulcher law[1], which introduces a phenomenological temperature associated to the magnitude of interparticle dipolar interactions. Fractional change of the peak temperature per decade of frequency[2] enlights the presence of interactions between particles in dilute liquids, along with a spin-glass-like state in powder samples, and remanence curves[3] show global demagnetizing behavior attributed to the combination of both spin surface disorder[4] and interparticle dipolar interactions. Nonetheless, exchange interaction between surface ions of different particles becomes more pronounced in the sample with the shortest interparticle distance, promoting an additive magnetizing effect[5].

[1] J Tholence, Solid State Commun. 35, 113–7 (1980)
[2] J L Dormann, L Bessais, D Fiorani, J. Phys. C: Solid State Phys. 21 2015–34 (1988)
[3] E P Wohlfarth, J. Appl. Phys. 29 595–6 (1958)
[4] J A De Toro *et al,* Chem. Mater. 29, 8258–68 (2017)
[1] C A M Vieira *et al*, J. Phys. Condens. Matter 31, 175801 (2019)

OC9

TiO_2-based photoanodes for solar-powered Hydrogen generation: controlled surface oxidation as a soft chemistry path towards water-splitting

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Climate change and our growing demand for energy pushes towards the development of alternatives to replace fossil fuels. H_2 is a promising fuel alternative, with only water as combustion byproduct, but the most used routes for obtaining it rely on fossil fuels, and others are costly or non-renewable. [1,2]

In this work, we develop TiO_2-based photoanodes (PAs) to harvest sunlight as energy source for water-splitting. We propose the controlled oxidation of Ti substrates through soft chemistry to obtain thin TiO_2 layers with optimized morphology, composition and crystallinity. The PAs were tested in two settings: a classic three-electrode photoelectrochemical (PEC) cell and a novel solid-state (SSPEC) cell, which allows us to split water vapor from air at room pressure and temperature. [3,4]

The photocurrent (PC) obtained for the classic PEC cells ranges from 0,5 to 1,2 mA (0V to 1V) in Na_2SO_4, pH7. For the SSPEC cells, the PC ranged from 5 to 40 μA at 80% RH and 1 to 10 μA at 40% RH (0V to 1,2V). This shows that we were able to improve TiO_2's PEC properties through a simple and cheap productive process under mild conditions. In addition, the use of metallic substrates with highly adhered oxide layers presents practical and environmental advantages compared to other assemblies. The SSPEC cell has great potential for H_2 production in deserted and/or off-grid areas.

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A. C. acknowledges funding from the Research Council of Norway (project nº 294681).

[1] P. Nikolaidis, A. Poullikkas, Renew. Sustain. Energy Rev 67, 597-611 (2017)
[2] Acar C., Dincer I., Int. J. Hydrogen Energ. 39 (2014)
[3] K. Xu *et al*, Photochem. Photobiol. Sci. 16, 10-16 (2017)
[4] K. Xu *et al*, Int. J. Hydrog. Energy 44, 2, 587-593 (2019)

OC10

ONE-POT SYNTHESIS OF TITANATE-TITANIA NANOHETEROSTRUCTURE: SYNERGISTIC MODIFICATION OF BAND STRUCTURE AND SURFACE PROPERTY FOR IMPROVED PHOTOCATALYTIC APPLICATION

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In order to combat groundwater pollution caused by harmful organic waste dumping, advanced oxidation processes (AOP) had been considered, where a suitable semiconductor species is irradiated, causing *in-situ* generation of reactive oxidative species (ROS), which oxidizes the pollutant to smaller, benign fragments. Owing to their structural and electronic properties, nanostructured titanium oxide (TiO_2)-based compounds are widely used as the heterogeneous photocatalyst [1]. Although layered titanate nanotubes (TiNT) have high specific surface area, unique disadvantage of it towards becoming a good photocatalyst is its weak photocatalytic activity due to fast recombination of the electron-hole pairs soon after generation. In order to rectify this, new anatase-TiNT heterostructures are being synthesized with retention of both adsorption and photocatalystic properties. As they have strong structural similarity with similar building blocks, they are easily interconvertible by low-energy-requiring pathways, realized by various post-synthetic treatment leading to partial TiNT-anatase phase transformation [2]. In this work, a very simple and economic one-step synthesis of a titanate-anatase nanostructure, titanate nanotubes decorated with small anatase nanocrystals (TiNT@AnNP), has been realized for the first time using a microwave-assisted alkaline hydrothermal method [3]. A systematic study has been carried out, varying the time and temperature, in order to achieve the best economical condition leading to most efficient catalyst [4]. They had been thoroughly characterized and a plausible in-situ anatase-TiNT transformation mechanism has been proposed. A water-soluble anionic dye Remazol blue (RB) is used as a model emerging groundwater contaminant to test the photocatalytic activity of these heterostructures under UV-visible light. Finally, in order to understand the AOP mechanism, a basic scavenger study was carried out with different types of inhibitors for possible ROS.

[1] Y. Zhang et al., RSC Advances, 5 (2015) 79479–79510.
[2] K. Cheng et al., Chem. Eng. J., 358 (2019) 1155–1165.
[3] S. B. S. Gusmão et al., J. Nanomaterials, 2019, Article ID 4825432.
[4] S. B. S Gusmão et al., Solid State Science, 2019 (In press).

OC11

MAGNETIC PROPERTIES OF CORE-SHELL Fe-Pt NANOPARTICLES IN IONIC LIQUIDS

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Most of nanoparticles properties differs from bulk either due to confinement or to the large portion of atoms at the surface. If smartly engineered, one can take advantage of the surface dependent properties to enhance the specific nanoparticles behavior for the desired applications. We present a recent work on the magnetic properties of stable core-shell Fe-Pt nanoparticles prepared by reaction of Fe(CO)5 and Pt2(dba)3 in 1-n-butylmethylimidazolium tetrafluoroborate (BMIm.BF4), hexafluorophosphate (BMIm.PF6), and bis(trifluoromethanesulfonyl)imide (BMIm.NTf2) under hydrogen [1]. The nanoparticles have a ultrasmall mean diameter around of 2 nm with a narrow size distribution. X-ray photoemission and absorption spectroscopies performed at the SXS and XAFS1 beamlines of the LNLS, respectively, put into evidence an oxidized Fe core wrapping a metallic Pt shell. The uncoordinated Pt ions at the nanoparticle surface displayed a strongly enhanced Pauli paramagnetism while the iron oxide core showed a Curie paramagnetism with diminished saturation magnetization.

[1] Janice Adamski *et al.* J. Phys. Chem. C 2018, 122, 4641−4650

OC12

SYNTHESIS AND CHARACTERIZATION OF CORE-SHELL (Au@Fe_3O_4) NANOSTRUCTURE

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Core-shell nanostructured materials of magnetite (Fe_3O_4) and Au are interesting for multifunctional applications in therapy and diagnosis such as hyperthermia using light and/or magnets [1,2]. To shed a light in this issue, in this work, core-shell nanostructures of Fe_3O_4 and gold were synthesized by the thermal decomposition method. X-ray diffraction data analysis confirms the formation of the spinel structure of the magnetite and the cubic phase of the metal gold, with lattice constants a= 8.38 Å for magnetite. An estimative of the crystallite sizes provide a D_{XRD}= 11.7 nm for the core-shell system. Data analysis of transmission electron microscopy indicates that the whole particle size is 14.2 nm; meanwhile, a size of 10.5 nm was determined from the micrographs for the core part. The careful analysis suggests that the shell region corresponds to the Fe_3O_4 with a mean width of 3.7 nm. On the other hand, UV-Vis spectroscopic measurements revealed the presence of bands corresponding to the magnetite phase (~201 nm). Moreover, a broad band centered at ~525 nm revealed a plasmon resonance band related to the nanometric size of gold in the core-shell structure. FTIR measurements evidenced the presence of Fe-O bonds (620 and 580 cm^{-1}) related to the Fe_3O_4 phase and bands located at 3415, 2920 cm^{-1} were related to –OH, C=C, respectively [3]. M vs. H curves indicated a superparamagnetic behavior for room temperature and blocked states at 5K. Meanwhile, Zero Field Cooled and Field Cooled measurements revealed a blocking temperature at Tb ~50K with an irreversibility temperature at Tirr ~ 215 K. The appearance of an unexpected peak was evidenced ~ 120 K, which was assigned to the Verwey temperature, which remains despite the fact that we have nano-sized particles. Additional studies are currently being carried out to better understand this problem. Additional studies are currently carried out to better understand this issue.

[1] Sadaphal, V.; Mukherjee, S.; Ghosh, S. Hybrid photomagnetic modulation of magnetite/gold-nanoparticle-deposited dextran-covered carbon nanotubes for hyperthermia applications. Applied Physics Express, v. 11, n. 9, p. 097001 (2018)

[2] León-Félix, L.; Sanz, B.; Sebastian., V.; Torres, T. E.; Sousa, M. H.; Coaquira, J. A. H.; Ibarra, M. R.; Goya, G. F. Gold-decorated magnetic nanoparticles design for hyperthermia applications and as a potential platform for their surface-functionalization. Scientific Reports. , v.9, p. 4185-1 - 4185-11 (2019)

[3] Khan, F. U. et al. Visible light inactivation of E. coli, Cytotoxicity and ROS determination of biochemically capped gold nanoparticles. Microbial pathogenesis, v. 107, p. 419-424 (2017)

OC13

Magnetorheological studies on aligned CNTs dispersed in magnetic fluid

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CNT based magnetic composites have been studied extensively pertaining to various potential technological applications like heat transfer, microwave absorbing materials, magnetic composites for drug delivery and magnetic force microscopy as nanoprobes[1-5]. In this work, we assess a method to decorate multiwall carbon nanotubes (MWCNT) with uniformly dispersed Fe_3O_4 nanoparticles (NPs) in kerosene called ferrofluid (FF). The samples were investigated for structural, morphological, magnetic and rheological properties. The average diameter of the MWCNT-Fe_3O_4 composites was 80 nm, however the average diameter of original MWCNT was 50 nm. The structural and morphological reveals that a thick layer of Fe_3O_4 NPs has been linked around the surface of MWCNTs. The viscosity shows a dependency on intensity of applied magnetic field. It may be attributed to that soft magnetic layer of Fe_3O_4 nanoparticles covering the surface of hollow MWCNTs and large length-diameter ratio of nanocomposites. Further, we modelled the aggregation features and sedimentation stability aspects of ferrofluid-MWCNT composite in fluidic form using extended DLVO approach.

[1]. W. Baaziz et.al, , *J. of Materials Chemistry A*, , 1, 13853-13861 (2013)
[2]. M. Zhu and G. Diao, *Nanoscale*, 3, 2748-2767 (2011)
[3]. B. Maddah and M. Hasanzadeh, Int. J. Nanosci. Nanotechnol., 13 (2), 139-149 (2017)
[4]. M.Chand et.al, US Patent, US9704628 B2 (2017)
[5]. M. Samadishadlou et.al, J. of artificial cells, nanomedicine, and biotech., 46(7), 1314-1330 (2018)

OC14

THERMAL DEPENDENCE OF COERCIVITY, IRREVERSIBILITY AND MAGNETIC ANISOTROPY IN FERRIMAGNETIC NANOPARTICLES

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Theoretical researches on magnetic properties of nanostructured magnetic materials are of wide interest of the scientific community due to the search for high performance technological applications. Nanoparticles (NPs) based on ferrimagnetic materials such as spinel ferrites are one the systems which have been drawing the most attention due to the possibility of tuning the magnetic properties by changing chemical composition and/or crystalline structure. In this work, we investigate the thermal dependence of coercivity for two ferrofluid samples composed by different sizes of core-shell $CoFe_2O_4@\gamma\text{-}Fe_2O_3$ NPs. These NPs were obtained by hydrothermal coprecipitation in alkaline medium and NP size was controlled by changing the synthesis medium. A subsequent hydrothermal surface treatment with $Fe(NO_3)_3$ produces the maghemite shell. The synthesized NPs have their chemical, structure and morphological properties characterized by Atomic Absorption Spectroscopy, X-Ray Diffraction and Transmission Electron Microscopy. Colloidal stability is checked by Small Angle X-Ray Scattering. For the magnetic characterization, first magnetization curves and zero-field cooled hysteresis loops are measured as a function of temperature. The coercive field is analyzed in the framework of the Stoner-Wohlfarth model. Our analysis also considers the size distribution and the temperature dependence of both magnetization and anisotropy constants, given that they affect the thermally activated transition from the blocked to the superparamagnetic (SPM) state. The model we propose adjusts the experimental data very well and allows us to predict the temperature dependence of the anisotropy field H_k. Then, we compare the predicted values with those extracted from the closure fields (H_{irr}) and from the first magnetization curves using the Law of Approach to Saturation (LAS). This comparison helps to shed light on the different sources of magnetic anisotropy, coming from the ordered core and the disordered shell, and their temperature dependence.

OC15

MAGNETIC IRREVERSIBILITY AND SATURATION CRITERIA IN ULTRASMALL BI-MAGNETIC NANOPARTICLES

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Ultrasmall magnetic particles are notorious for exhibiting a magnetization increase even at quite intense applied fields, behavior which can be interpreted as a non-saturation of the magnetic disordered shell even if the nanoparticle magnetization is reversible. In this work we study two kinds of ultrasmall core@shell nanoparticles (3 nm) with contrasting core anisotropy, composed of $MnFe_2O_4$ and $CoFe_2O_4$ cores covered by a thin maghemite layer. In order to investigate the saturation criterion associated to the closure of major loops (in contrast to minor loops), we use several procedures to determine, at moderate fields, if the effective anisotropy energy barrier is overcome or not. Firstly, we carefully evaluate the closure field of the hysteresis loop, interpreted as the effective anisotropy field, correspondent to two different contributions. One, arising from the nanoparticle core, is related to the coercivity and the other one being associated to pinned spins of the nanoparticle shell. Secondly, the ZFC-FC magnetization measurements taken at different fields give us information about both the anisotropy energy barrier distribution and the thermal dependence of effective anisotropy field. Thirdly, forced minor loops are performed, measured after either ZFC or FC processes, to counter-check the effective magnetic anisotropy at low temperature of both samples. Finally, we perform major hysteresis loop calculations in order to better understand the magnetization processes involved. To go further, we propose in this study a procedure to extract information about the two contributions which composes the effective magnetic anisotropy field.

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POSTERS

P1

MAGNETIC AND STRUCTURAL PROPERTIES OF COBALT FERRITE NANOPARTICLES DOPED WITH ZINC AND NICKEL

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Magnetic spinel ferrites with general chemical formula $M_xFe_{3-x}O_4$ (where M = Co^{2+}, Ni^{2+}, Mn^{2+}, Zn^{2+}, and x = 0−1) in form of nanoparticles (NPs) have great potential in tunability of their magnetic properties by vary of their size and chemical composition [1–3]. Magnetization saturation (M_S) and coercivity force (H_C) of magnetic NPs are strongly correlate with their chemical composition. Spinel ferrites consist of two antiferromagneticaly ordered sublattices: the tetrahedrally and octahedrally coordinated A- and B-sites. According to Néel's model the spinel is ferrimagnet with net magnetic moment because of non-equality of magnetic moments of two sides $\mu = \mu_a - \mu_b$. The A-sides filled by divalent cations in case of normal spinel while in the inverted spinel A-sides are filed with the trivalent cations but B-site filled by half with both cations. In frame of this work, the set of cobalt ferrites NPs doped with different content of zinc (0 μ_B) or nickel (2 μ_B) was prepared with sol-gel self-combustion rout. Structural and morphological features of particles were studied with XRD, STEM and EDX techniques. Prepared particles demonstrated a crystalline nature with the monotonical distribution of the elements and distribution of size in range of 17−29 nm. Obtained particles demonstrate well tunable magnetic properties with the high values of saturation magnetization and coercivity, which strongly depend on chemical composition. It was demonstrated that small adding ($x < 0.25$) of nickel or zinc allows to increase room temperature M_S values up to 69±3 Am^2/kg for $Ni_{0.25}Co_{0.75}Fe_2O_4$ and 74±2 Am^2/kg for $Zn_{0.25}Co_{0.75}Fe_2O_4$. This increase was explained by non-equilibrium cation distribution because of that part of Fe^{3+} (5 μ_B) cations with highest magnetic moment migrate to octahedral sides. Subsequent increase of their content leads to both decreasing of saturation magnetization and coercivity.

[1] Silva, F. G. da et al., J. Nanosci. Nanotechnol. 19, 4888–4902 (2019)
[2] Mameli, V. et al., Nanoscale 8, 10124–10137 (2016)
[3] Muscas, G. et al., J. Alloys Compd. 796, 203–209 (2019)

P2

Tuning long-range functionals for determining reorganization energies of photosynthetic systems

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Photosynthetic systems convert solar energy, absorbing it from light through a set of organic molecules such as carotenoids and chlorophyll. It is important to understand the mechanisms of photosynthesis because it is the most abundant manner of solar energy conversion in nature. For this reason, it is necessary to investigate the mechanisms of transport of energy. The reorganization energy is the energy cost for changing the geometry of a molecule from neutral to charged. This quantity is necessary to understand the mechanisms of transport of energy. To simulate the reorganization energy one can carry out density functional theory (DFT) computations [1]. To avoid delocalization of the systems wave function, which is a well-known tendency of traditional DFT, this often requires long-range corrected functionals (LRCF) such as CAM-B3LYP, LC-BLYP, and wB97 for more accurate results. LCRF consists, among other concepts, on partitioning the Coulomb operator into short-range and long-range components using standard error function with separation parameter w [2]. In this work, we show a procedure for tuning the separation parameter (w) and how this procedure impact the calculations of the reorganization energy in this kind of systems.

[1] Da Silva Filho, Demetrio & Coropceanu, Veaceslav & Gruhn, Nadine & Neto, Pedro & Brédas, Jean-Luc. (2013). Intramolecular reorganization energy in zinc phthalocyanine and its fluorinated derivatives: A joint experimental and theoretical study. Chemical communications (Cambridge, England). 49. 10.1039/c3cc42003e.
[2] Lima, Igo & Prado, Andriele & Martins, João & Neto, Pedro & Ceschin, Artemis & Cunha, Wiliam & Da Silva Filho, Demetrio. (2016). Improving the Description of the Optical Properties of Carotenoids by Tuning the Long-Range Corrected Functionals. The journal of physical chemistry. A. 120. 10.1021/acs.jpca.5b12570.

P3

ADSORPTIVE REMOVAL OF PHOSPHORUS BY CORE-SHELL BIMAGNETIC NANOPARTICLES

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Phosphorus (P) is an essential nutrient to maintain life in water bodies, although, in high concentrations, it may cause eutrophication of aquatic environments. In order to avoid this phenomenon, P must be removed from wastewaters before its discharge, since a significant amount of P can be found in wastewaters [1]. Thus, this work aims to investigate the P removal from aqueous solution through P adsorption by core-shell bimagnetic nanoparticles ($CoFe_2O_4@\gamma\text{-}Fe_2O_3$). A hydrothermal coprecipitation in alkaline medium followed by a surface treatment was the methodology applied for the synthesis of the nanomaterial. X-ray diffraction measurements, transmission electron microscopy, BET surface area analysis and magnetization measurements were performed to characterize the nanomaterial. Batch adsorption tests using aqueous solution of P provided information regarding the influence of solution pH, contact time, initial concentration of P, and temperature on the adsorption. In addition, batch adsorption tests with secondary wastewater effluent were also carried out to evaluate the influence of others compounds on the adsorption. The pH effect study confirmed that the electrostatic interactions between the adsorbate and the adsorbent are favored the lower the pH is. The Elovich model best fits the kinetics data. The equilibrium was achieved within three hours. The Freundlich model best fits the equilibrium data, suggesting that multilayers are formed and that the adsorbent surface is heterogeneous. The thermodynamic analysis indicates that the process is spontaneous, endothermic and that the disorder in the solid/solution interface increases due to the P adsorption onto the adsorbent surface. The nanomaterial presented a great performance with the sample of secondary wastewater effluent.

[1] W. Verstraete et al., Bioresource Technology, 100, 5537-5545, (2009)

P4

SYNTHESIS OF MAGNETIC NANOPARTICLES EMBEDDED IN A LAPONITE DISPERSION

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In this work magnetic nanoparticles (MNp) were synthesized in an environment of nanostructured dispersion of Laponite (Lp) nanoclays [1], [2], with the objective to create a new class of smart materials exploiting the best characteristics of each individual part. The magnetic particles are largely employed in technological and biomedical applications such as cancer treatment, via hyperthermia [3], [4], for example, drug delivery and cell separation. Due to its high purity, optical transparency and the excellent stability of its dispersions laponite [5], [6] was used as a controlled medium of magnetic particle synthesis. The produced material was characterized by Powder X-ray Diffraction (XPD - LNLS), Small Angle X-ray Scattering (SAXS), Transmission Electron Microscopy (TEM) and Fourier-Transform Infrared Spectroscopy (FTIR). The presented results reinforce this new nanocomposite as a promising material for medical and technological applications.

[1] C. B. Kern. Universidade de Brasília-UnB, 2016.
[2] V. Tzitzios *et al.J. Mater. Chem.*, vol. 20, no. 26, p. 5418, 2010.
[3] G. F. Goya, V. Grazu, and M. R. Ibarra, *Curr. Nanosci.*, vol. 4, no. 1, pp. 1–16, 2008.
[4] S. K. Sharma, Surender Kumar (Ed.) Springer. 2017.
[5] H. Z. Cummins,*J. Non. Cryst. Solids*, vol. 353, no. 41–43, pp. 3891–3905, 2007.
[6] B. Ruzicka, and L. Zulian, and G. Ruocco” 2005.

P5

L-LYSINE COATED MAGNETIC NANOPARTICLES FOR ASA REMOVAL FROM AQUEOUS SOLUTIONS

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Pharmaceutical residuals have been classified as emerging pollutants, i.e. they are not routinely monitored and may cause adverse effects in environmental and human health [1]. To remove these pollutants from wastewater, conventional methods such as reduction, precipitation, adsorption, oxidation and ion exchange are commonly used [2]. However, some methods based on magnetically assisted chemical separation have been proposed to be cleaner and more efficient. In this study, we investigate the removal of acetyl salicylic acid (ASA) from aqueous solutions using magnetic nanoadsorberts based on ferrite nanoparticles (NP) modified with L-lysine. The nanoadsorbents were synthesized using the hydrothermal coprecipitation method in alkaline medium followed by a surface treatment with $Fe(NO_3)_3$ leading to a $CoFe_2O_4@^{\gamma}\text{-}Fe_2O_3$ core-shell NP. The surface modification was carried out by stirring the NP and the L-lysine at pH = 11.5 for 45 min. The influence of time, solution pH and initial ASA concentration were evaluated from batch studies using 1.3 g/L of the nanoadsorbent. After chemical adsorption, the NP were separated using a hand-held magnet and the final concentration of ASA in the decanted solution was determined by UV-VIS spectroscopy at 220 nm. The results of the batch studies were analyzed in the framework of Langmuir and Freundlich models in order to evaluate the maximum adsorption capacity and the extent of the affinity. Finally, the kinetics data were analyzed with pseudo-first order and pseudo second-order models.

[1] J. I. MacRae, S. F. Owen, L. P. Barron, N. R. Bury, T. H. Miller Environ. Pollut., 239, 129 (2018)
[2] H. Sadegh et al., , J. Nanostructure Chem., 7, 1 (2017)

P6

Investigation of the magnetic properties of cobalt, zinc and copper mixed ferrite nanoparticles

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Magnetic ferrite nanoparticles (NPs) have attracted considerable attention of scientific community of different areas for many years. This interest is attributed to their structural, electrical, optical and magnetic properties that lead to novel technological and biological applications such as magnetic fluids, nanoeletronics, magnetic optical devices and magnetic biomedical applications. We currently elaborate ferrite based NPs in order to disperse them in water [1]. In this context, we have synthesized NPs based on Co0.5Zn0.25Cu0.25Fe2O4 mixed ferrite. This NPs are obtained by hydrothermal coprecipitation in alkaline medium followed by a surface treatment that creates an iron-rich surface layer. NPs chemical composition is checked at each step of the synthesis by using atomic absorption spectroscopy and their structure investigated by X-Ray Diffraction (XRD) experiments realized on powder samples. Transmission Electron Microscopy (TEM) pictures show their morphology and allow a mean size determination, which well matches the one deduced from XRD analysis. Low field and high field DC magnetization experiments are combined with hysteresis loops measurements to characterize powders and liquid samples. Then, we extract the thermal dependence of both saturation magnetization and coercivity of nanoparticles. The temperature dependence of magnetization is explained in the framework of Bloch's law and the coercivity is compared to the Kneller's law. The produced nanoparticles present very high saturation magnetization values, as well as coercivity, making them promising candidates for several applications.

[1] J. A. Gomes, M. H. Sousa, F. A. Tourinho, R. Aquino, G. J. da Silva. J. Depeyrot. E. Dubois, R. Perzynski, J. Phys. Chem. C 112 6220 (2008)

P7

ON WATER CLUSTERS CIS-TRANS STRUCTURES PROPERTIES

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In this work, we investigate the stability of small water clusters when placed under a uniform electric field and analyze some of the properties of these systems, such as the orientation of the water molecules in relation to the external electric field and in relation to themselves.

Water has an intrinsic dipole momentum; thus water molecules reorient themselves when an external electric field is placed. For each water cluster studied (dimer, trimer and tetramer), an electric field of intensities $0.001 au$ to $0.01 au$ was applied, where ($1au=512.2V/nm$). These electric fields were reported in graphene sheet experiments.

For specific values of the electric field intensity, we observe structural phase transitions in the clusters and compared the molecular arrangements before and after the transition. The results indicate that each cluster needs a specific electric field intensity in order to change its arrangement.

[1] B. Delley, J. Chem. Phys. 92, 508-517 (1990).
[2] B. Delley, J. Chem. Phys. 113, 7756-7764 (2000).
[3] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864-B871 (1964).
[4] W. Kohn and L.J. Sham, Phys. Rev. 140, A1133-A1138 (1965).
[5] J.P. Perdew and Y. Wang, Phys. Rev. B 45, 13244-13249 (1992).
[6] J.P. Perdew, K. Burke and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996)
[7] A.D. Becke (1993). J. Chem. Phys. 98 (2): 1372–1377

P8

Magneto hyperthermia of core/shell (γ-Fe_2O_3@$CoFe_2O_4$) Nanoparticles: the effect of shell thickness.

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Within the nanomaterials research, magnetic nanoparticles (NPs) have aroused high interest due to their great technological potential, with a promising future in diverse applications, with a great appeal in biomedical applications. We can highlight its use in the targeting of drugs, contrast agents in nuclear magnetic resonance, and magneto hyperthermia. In this work we obtained Core-Shell magnetic NPs with the formula γ-Fe_2O_3@$CoFe_2O_4$, with different shell thicknesses. In these NPs the magnetic properties can be related to the coupling between soft and hard magnetic phases, raising the possibility of the appearance of magneto thermal properties of interest [1]. Using the bottom-up synthesis method [2], nanoparticles of Fe_3O_4 magnetite were obtained by precipitation in an inert atmosphere of a mixture of solutions of Fe^{3+} and Fe^{2+} salts in alkaline medium. A hydrothermal chemical treatment [3] with Co^{2+} salt solution in an atmosphere of O_2 with different concentrations and pHs, promotes the formation of the superficial cobalt ferrite layer, with different thicknesses, and oxidize the magnetite to maghemite. The structure and morphology are studied by X-ray diffraction and transmission electron microscopy (TEM), the nanoparticles have spinel structures and the diameter (Drx) is determined by the Scherrer formalism. Chemical composition was obtained by atomic absorption spectroscopy (AAS) and using the Drx values it was possible to calculate the thickness of the $CoFe_2O_4$ layer. Measurements of magnetometry were performed by using a quantum design PPMS, at room temperature and at 5 K with applied fiels up to 9 T. The results indicate that NPs behave as uniaxial monodomains, presenting Hc greater than pure magnetite, indicating an increase of magneto crystalline anisotropy with increasing thickness of the $CoFe_2O_4$ layer. Magneto hyperthermia measurements were performed using the DM5 Series Nanoscale Biomagnetics, in adiabatic condition at the concentration of 0.5 mg/mL of magnetic material, with AC magnetic field amplitude of 300G and at a frequency of 760 Hz. The heating efficiency is expressed through specific power absorption (SPA) values, and shows a small decreasing on SPA values with the decreasing of $CoFe_2O_4$ shell amount.

[1] Lee, J-H. *et al.; Nature Nanotechnology*, vol 6, 2011, 418-422.
[2] Massart, R.; *IEEE Trans. on Magn*., **17**, 1247, 1981.
[3] Tourinho, F. A.; Depeyrot, J.; Silva, G. J.; Lara, M. C. F. L.; *Braz. J. Phys*. **28**, 413, 1998.

P9

TOWARDS THE CONTACT-FREE MEASUREMENT OF LARGE SHEET RESISTANCES

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The sheet resistance of thin conducting films and coatings is an important measure for quality assurance. However, the analysis of films based on novel materials may pose a challenge to the established measuring techniques. Ultrathin inorganic nanomaterials as well as conducting plastics are two examples. Both material classes lead to largely increased sheet resistance values, either due to a significantly decreased film thickness or increased bulk resistivity. Fourpoint probes are not appropriate since neither the mechanical probe contact to the film nor the required very low current source can be established reliably. In the current brief, we assess as alternative various contact-free sheet resistance measurement techniques based on the induction of eddy currents [1,2]. The methods differ by the way how the eddy current flow in the film is detected in the inducing primary circuit. The sensitivity is analyzed for detecting eddy currents in PEDOT:PSS films [3] by off-balancing bridge circuits or measuring the power absorption of different oscillator circuits. Finally, the frontier between eddy current based methods and capacitive techniques is addressed.

[1] G. Miller, D. Robinson, J. Wiley, Rev. Sci. Instrum. 47 (7) 799 (1976)
[2] J. Krupka, Meas. Sci. Technol. 24, 062001 (2013)
[3] D. Mantione, I. del Agua, A. Sanchez-Sanchez, D. Mecerreyes, Polymers 9, 357 (2017)

P10

STUDY OF SnO THIN FILMS GROWN BY MBE FOR SnO/SnO_2 *p-n* JUNCTION FORMATION

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Tin monoxide (SnO) is considered one of the most important *p-type* semiconductor oxides available nowadays. The *p-type* conductivity originates from Sn vacancies, because the equilibrium concentrations of defects of Sn interstitial and O vacancy are low, and not enough to compensate holes generated by Sn vacancies [1]. It has a tetragonal unit cell and indirect bandgap in the range 2.5-3.4 eV. SnO thin films have very high hole mobility values (about 7 cm^2/Vs), and the hole density in these films is about 10^{15}-10^{19} cm^{-3}, which can be obtained only by controlling deposition parameters, thus offering great potential for the modern electronic and optoelectronic device manufacture [2]. SnO thin films are normally deposited by rf-magnetron sputtering, pulsed laser deposition or microwave irradiation method. The great novelty of this work is the deposition method of this material: SnO thin films were grown by molecular beam epitaxy (MBE), for posterior coupling with sol-gel SnO_2 (tin dioxide) nanostructured thin films, thus forming a SnO/SnO_2 *p-n* junction. Initial transport results showed *p-type* conductivity and different mobility values for SnO grown in different kinds of substrate: 1.4±0.2 cm^2/Vs (YSZ substrate), with sheet resistance of 24 kΩ; 0.8±0.4 and 1±0.2 cm^2/Vs (on sapphire (0001) with different parameters of deposition, as the deposition time), with sheet resistance of 160 and 100 kΩ, respectively. X-ray diffraction results exhibited tetragonal SnO peaks, and the Fourier transform infrared spectroscopy (FTIR) showed absorption peaks: in the range 495-534 cm^{-1}, which is ascribed to the stretching vibrations of Sn–O, and in 742 cm^{-1}, related to O–Sn–O bonds.

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[1] A. Togo, F. Oba, I. Tanaka, Phys. Rev. B 74, 195128 (2006)
[2] K. J. Saji, Y. P. V. Subbaiah, K. Tian, A. Tiwari, Thin Solid Films 605, 193 (2016)

P11

Organoclay Preparation and Characterization Aiming Wastewater Treatment Applications

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Over the past few years, several scientific works have been dedicated to the preparation and study of composite materials that combine rigid components with soft and flexible materials aiming potential applications in biomedicine and materials engineering. In particular, mineral clays have been considered as fundamental components in the preparation of systems for drug encapsulation, removal of contaminants in water and biocompatible materials for implants [1]. In our work we propose the synthesis of an organoclay capable of removing of inorganic and organic contaminants from wastewater. We prepared and characterized novel montmorillonite-organoclays using a commercial nonionic surfactant, Simulsol M45, by Seppic. This surfactant presents a lamellar phase, composed of a regular stack of amphiphilic molecules bilayers separated by water layers, which is particularly interesting as a template because the clay nanoparticles can be incorporated to either the water channel or the bilayer, depending on their character, hydrophilic and hydrophobic, respectively [2]. The confinement of the clay platelets is modulated by controlling the water content of the lamellar phase. Since the surfactant is nonionic, the main mechanism involved in the formation of a stable structure is of entropic nature, i.e. thermal fluctuations. We investigate the original compounds by transmission electron microscopy (TEM), small angle X-ray scattering (SAXS) experiments, dynamic light scattering (DLS) and Zetammetry. The SAXS experiments were also used for the characterization of the structural properties of the prepared organoclays. Finally, the adsorption capacity of the organoclays were investigated by FAAS and UV-Vis techniques.

[1] CARRETERO, M. I.; LAGALY, G. Applied Clay Science, v. 36, 1-3 (2007).
[2] CONSTANTIN, D.; DAVIDSON, P. ChemPhysChem, v. 15, 1270-1282 (2014).

P12

QUANTUM PHENOMENA IN NANOSCALE TRANSISTORS WITH MULTIPLE GATES

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The semiconductor industry integrates routinely billions of nanoscale transistors into electronic circuits. Although microelectronics evolutionary evolved into nanoelectronics over the last two decades, also completely novel device concepts emerge at the nanoscale. One of such emerging concepts suggests controlling the charge density along the semiconducting transistor channel via various independent program gates [1,2]. Since impurity doping of ultrathin channel materials becomes unreliable, such electrostatic charge control is attractive and allows to configure device operation via electrical signals during run time. The spatial modulation of the semiconductor band structure leads to interesting quantum phenomena affecting the charge transport via discretization of electronic states and charge tunneling. In the current brief, we apply the non-equilibrium Green's function method to quantify the impact of these quantum phenomena based on given band diagrams of multiple-gate nanoscale transistors. Band-to-band tunneling effects were accounted for employing an effective potential. For representative potential profiles, the spatial and energetic distributions of the electronic states are determined in the form of the total and partial local densities of states detailing the contribution of each contact separately. The current through the nanoscale transistor is parametrized by a transmission coefficient, which shows quantum resonance and tunneling signatures. Finally, the brief concludes with a brief discussion of the impact of the charge carrier effective mass and the injection gap on the transistor operation.

[1] S. Blawid, D. de Andrade, S. Mothes, M. Claus, *IEEE J. Electron Devices Soc.* 5, (6), 473 (2017)
[2] R. Moura, N. Tiencken, S. Mothes, M. Claus, S. Blawid, *IEEE Trans. Nanotechnol.* 17 (3), 467 (2018)

P13

SIZE AND SHAPE EFFECTS ON THE HYPERTHERMIA PERFORMANCE OF Bi-MAGNETIC CORE / SHELL NANOPARTICLES

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Localized magnetic particle hyperthermia, namely the heating dissipation of magnetic nanoparticles (MNPs) under the application of alternating magnetic field, is a promising tool for cancer treatment with minima side effects. Recently, a lot of research activity is focused on improving the heat power as it is measured through the Specific Absorption Rate (SAR) by modifying the size, shape or the morphology of MNPs. Notably, bi-nanoparticles of core/shell morphology give higher SAR values than the single-phase oxides. [1, 2]
We study the mechanism of magnetic hyperthermia for superparamagnetic ferrimagnetic nanoparticles and bi-magnetic nanoparticles with ferromagnetic (FM) core/ ferrimagnetic (FiM) shell morphology. We have developed a phenomenological model in the framework of the linear Néel-Brown relaxation model to calculate the SAR of complex soft Fe/ hard Fe_3O_4 nanoparticles for different core sizes, shapes and surfactant thickness [3]. We have simulated Their magnetic behaviour has been studied with the Metropolis Monte Carlo simulations technique.
Our calculations show that for all the sizes and shapes the bi-magnetic FM/FiM nanoparticles give higher SAR values than the pure ferrimagnetic ones due to their higher core saturation magnetization. Maximum SAR value is obtained for the truncated cuboctahedral shape of the nanoparticles. The decrease of the surfactant thickness results in an increase of the SAR values in all cases. Our results are in agreement with the available experimental data from Fe/Fe_3O_4 nanoparticles, confirming that the complex nanoparticles with core/shell morphology optimise the heating properties for hyperthermia.

[1] C. Binns, P. Prieto, S. Baker, P. Howes, R. Dondi, G. Burley, L. Lari, R. Kröger, A. Pratt, S. Aktas, J. K. Mellon, *J. Nanopart. Res.* **14** (2012) 1136.
[2] Seung-hyun Noh, Seung Ho Moon, Tae-Hyun Shin, Yongjun Lim, Jinwoo Cheon, *Nano Today* **13** (2017) 61–76.
[3] M. Vasilakaki, C. Binns, K. N. Trohidou, *Nanoscale* **7** (2015) 7753-7762.

P14

Wrinkling evolution of tantalum films sputter deposited on PDMS substrate under uniaxial strain

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The comprehension and control of wrinkling properties of flexible polymers-supported metallic films are challenging topics on the flexible electronic materials, being the subject of theoretical and experimental investigations for several decades [1]. In this context, interfacial adhesion between the metallic film and the polymer surface have attracted a remarkable amount of interest due the possibility of controlling them by using specific deposition parameters, which can be exploited in the development of many high-tech fields such as microelectronics systems, optic devices, flexible electronic and sensors [2].

In this work, tantalum (Ta) films have been deposited on elastic polydimethylsiloxane substrate by magnetron sputtering technique. For comparison, films of tantalum have been also deposited on polyimide (kapton). The wrinkling patterns are investigated by using optical microscopy, atomic force microscopy, scanning electron microscopy. The experiment shows that the as prepared Ta-films on PDMS spontaneously forms periodic horizontal wrinkles and parallel perpendicular cracks due to the residual thermal stresses stored up during and after film deposition.

Uniaxial stretching tests along the samples are then carried out to determinate the evolution of wrinkles and cracks density. The external stretching has expended the existing winkles, then their periodicity and with increasing the strain, new cracks appear perpendicular applied strength (longitudinal direction). The experimental results show a significant coupling effect between the cracking mechanisms for metallic film deposited on PDMS and applied strain.

The structural characteristics, morphological evolutions and physical mechanisms of these wrinkling patterns have been besides discussed and analyzed based on the stress theory.

[1] C. K. Tee Benjamin, O. Jianyong, Adv. Mater. 30, 1802560 (2018)
[2] W. Wu, Sc. Technolo. Adv. Mat., 20:1, 187 (2019)

P15

Modeling Exciton Diffusion in Crystalline Chromophore Assemblies

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Exciton diffusion is a process of great importance in the working of optoelectronic devices and photosyntetic systems. Attempts to control exciton diffusion have been made focusing on molecular engineering and on the architecture of the assembled chromophores. In this context, metal organic frameworks (MOFs) have been employed to produce organized structures in which exciton transfers can be channeled to a single direction [1]. Furthermore, structures may be developed combining two different molecules, affecting exciton dynamics in the system In this work, we perform theoretical calculations to determine the efficiency of exciton transfers on donor-acceptor MOFs composed of 4,4′-(anthracene-9,10-diyl)dibenzoic acid (ADB) and ((2,5-bis(butyl)-3,6-bis(4-carboxylicphneyl-4-yl)-2,5-dihydropyrrolo[3,4-*c*]pyrrole-1,4-dione (DPP). We employ density functional calculations to simulate absorption and emission spectra of these compounds and make use of a protocol [2] to estimate exciton transfer efficiency and diffusion length in these materials. Finally, we simulate exciton dynamics for different relative concentrations of donors and acceptors by means of a Kinetic Monte Carlo model and compare our results with experimental data [2].

[1] DE SOUSA, Leonardo Evaristo et al. Fast predictions of exciton diffusion length in organic materials. **Journal of Materials Chemistry C**, v. 7, n. 14, p. 4066-4071, 2019.
[2] HALDAR, Ritesh et al. Anisotropic energy transfer in crystalline chromophore assemblies. **Nature communications**, v. 9, n. 1, p. 4332, 2018.

P16

Virtual Screening and Quantum-Chemical Study of the prediction pKa's Sulfa-like Compounds

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Sulfonamides group are important broad-spectrum antibiotics used globally, some medicines approved to FDA and others were used as a starting point for synthesizing new drugs both theoretically and experimentally. pKa's sulfa molecules are important for understanding their chemical properties and applications in medicine using virtual screening, drug-design, and others. The experimental determination of pKa's is not always easy because of problems such as interference from other solutes in complexity due to the solvent system, difficulties in isolation of specific residues, complex substrate environment, etc[1]. Hence, prediction pKa's using chemical techniques has been growing recently. Furthermore, some studies compare protocols to calculation pKa's small molecules. In this work, we perform theoretical calculations, with 12 different functionals and 10 distinct basis sets, to calculation pKa's values to sulfachloropyridazine. We observe differences less 0.28 units' pKa compared theoretical and experimental. Then, using different parameters of Virtual Screening we found other 10 molecules, with a similarity parameter is always greater than 0.7. Were calculated pKa value with the same functional and basis set and compare it with experimental data for all new molecules. So, we compared different parameters used to virtual screening used to calculation pKa. Finally, we obtained electronic properties to made correlations with pKa through Principal Component Analysis.

[1] THAPA, Bishnu; SCHLEGEL, H. Bernhard. Density functional theory calculation of pKa's of thiols in aqueous solution using explicit water molecules and the polarizable continuum model. The Journal of Physical Chemistry A, v. 120, n. 28, p. 5726-5735, 2016.

P17

STUDY OF NANOPARTICLE STRUCTURE ON PH-DEPENDENT FERROFLUID PHASE TRANSITION BY MEANS OF MONTE CARLO SIMULATION

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The stability of magnetic colloidal dispersion (ferrofluids) depends on the balance between attractive interactions (magnetic and van der Waals), which tend agglomerate the colloidal particles, and the repulsive ones, which tend to set them apart. The repulsion usually comes from surfactant or charge density on the particle surfaces. The pH of the ferrofluid is a major factor affecting particle surface charge and thus particle agglomeration. Sol-gel phase transitions have been observed in cobalt ferrite nanoparticles dispersed in water with variable pH [1, 2]. In this work, the dependence of surface charge on pH was modeled by means of the so-called “2-pK charging model”, which describes a charging process that depends on two subsequent chemical reactions. The simulation was performed by means of the Metropolis algorithm with the energy of interaction being formulated by means of an extended DLVO theory (X-DLVO) and the 2-pK model. We analyse the results of the simulations through the pair correlation function and the structure factor, which evidentiate the formation of particle structure as pH changes from acidic to neutral, as with empirically observed sol-gel transitions.

[1] Campos, A. F. C., et al Brazilian Journal of Physics, 39:230–235 (2009).
[2] Campos, A. F. C., et al EPJ: E, Soft Matter, 36:1–11 (2013).

P18

EXCITON DENSITY EFFECTS IN ORGANIC MATERIALS: DIFFUSION LENGTH, LIFETIME AND QUANTUM EFFICIENCY

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When it comes to organic electronics, devices such as Organic Photovoltaics (OPVs) and Organic Light-Emitting Diodes (OLEDs) exciton dynamics play an essential role. For singlet excitons, the diffusion process happens via a process known as Förster Resonance Energy Transfer (FRET) [1]. Such process is a non-radiative energy transfer mechanism, in which the excitation energy from a donor molecule migrates to an acceptor one. The rate for which this kind of transfer occurs depends on exciton lifetime and the so called Förster radius. In this work we perform simulations of exciton diffusion via a Kinetic Monte Carlo (KMC) model that includes exciton-exciton annihilation phenomenon, which affects the efficiency in energy transfer[2]. To understand the effects of exciton concentration in diffusion length, we performed simulations considering Förster radii ranging from 20 Å to 40 Å and exciton lifetimes from 500 ps to 5000 ps. Exciton concentrations, measured in excitons per lattice site, varying from 0.1% to 4.9% were examined. We were able to obtain a relationship between critical concentrations for which annihilation effects hinder device efficiency and Förster radii, which allowed for the connection between our results and actual materials employed in optoelectronic devices[3]. We were able to provide a linkage between our results and experimental conditions by comparison with pump fluences. Furthermore, we showed how exciton concentration is able to affect exciton diffusion length. Finally, we trace these effects to significant reductions in average exciton lifetime.

[1] Förster, T. Annalen der physik, 437, 55, (1948).
[2] Sousa, L. *Chemistry of Materials* 31.17 (2019)

P19

Dynamics and Rovibrational Spectroscopy of Weakly Bonded Complexes

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Using experimental techniques in the dissociation of multiples photons and induced fluorescence, Ashfold et al. [1] measured reaction rate to remove methylene (CH2) from noble gases (He, Ne, Ar, Kr, Xe) and others molecules N2, H2, O2, CO, and CH4. This study showed the high efficiency of argon to remove CH2. Such experiments were performed at low pressure. This condition is more adequate for future applications. These results suggest that mainly step to remove CH2 for noble gases was responsible by intersystem crossing singlet-triplet ruled by long-range attractive forces (van der Waals). Therefore, these results have been interesting to the scientific community because of the role of such processes in the photochemical reaction system [2]. Even though/despite methylene is applied in wide technologies, its properties are not fully established yet [3]. Accordingly, complexes formed by methylene and noble gases are good candidates to investigate hydrogen bound behavior in different conditions. In this work, we performed the dynamic of complexes constituted of methylene and noble gases - Ng (Ng = He, Ne, Ar, Kr, Xe e Rn). Through a quantum chemistry computational procedure, we obtained rovibrational energies, spectroscopic constants and lifetime of complex interactions as a function of temperature for all Ng aforementioned. It was observed that the CH2-He system shows a shallow potential with no rovibrational levels and a lifetime of around 1 ps. This short lifetime shedlight an unstable behavior. On the other hand, the CH2-Rn complex was the one that presents the deepest potential well. Hence, this complex reveals many rovibrational levels, exhibiting a stable behavior, as a greater lifetime.

[1] Ashfold, M. N. R.; Fullstone, M. A.; Hancock, G.; and Ketley, G-W; Chem. Phys. 1981, 245.
[2] Bley, U.; and Temps, F. J. Chem. Phys. 1993, 98, 1058.
[3] Laufer, A. H.; Rev. Chem. Int. 1981, 4, 225; Langford, A. O.; Hrvoje, P.; and Moore, C. B.; J. Chem. Phys. 1983, 78, 6650.

P20

ROLE OF SIZE, MORPHOLOGY, SURFACE COMPOSITION ON MAGNETIC VORTEX STATE AND HYPERTHERMIA PROPERTIES OF IRON OXIDE NANOPARTICLES

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The present work report the synthesis of α-Fe_2O_3 nanoparticles by microwave-assisted hydrothermal route by varying the ratio of sodium phosphate to sodium sulfate in a controlled fashion and their subsequent annealing in reducing environment [Ar (96 %) + H_2 (4%] to tune their size, morphology and phase composition. A clear growth of nanostructures, nanotubes, nanorods and nanodiscs is observed with the increase in concentration of phosphate ions in contradiction of previous reports. Contrary, the metallic iron phase decreasing gradually from 15 % to 0% with increasing the concentration of phosphate ions. An interesting trend in so called magnetic Verwey transition and its dependence on bulk magnetite and concentration of phosphate on the nanoparticle surface indicating the loss of stoichiometry from nanotubes to nanodiscs. We proposed a unique model to explore it through several experimental techniques namely X-ray diffraction, advanced electron microscopy, Fourier transform infrared spectroscopy, Mossbauer spectroscopy, and dc magnetic measurements. Interestingly, a sharp drop in coercivity values from nanotubes to nanodiscs indicated the presence of magnetic vortex state for nanodisc, which is subsequently confirmed through Lorentz microscopy and micromagnetic simulations data. Finally, we have performed the magnetic hyperthermia experiment (450 Oe and 100 kHz) to see specific absorption rate (SAR) for these nanoparticles. The observed value for nanodisc is rather low ~ 3.5 W/g in comparison to that obtained from micromagnetic simulation (~ 7 W/g), which is probably due to large size of nanodisc i.e. 745 nm or due to alignment of nanodisc in suspension during the experiment.

Key Words: Ferrimagnetic iron oxide nanoparticles, Verwey transition, stoichiometry, magnetic hyperthermia

P21

Dispersion of $CoFe_2O_4$ functionalized nanoferrite into a Deep Eutectic Solvent

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Magnetic nanoparticles are materials produced for various applications, such as in the cosmetic, aeronautical, pharmaceutical and medical industries. Magnetic nanocoloids are stable dispersions of magnetic nanoparticles dispersed in a specific carrier liquid [1] The different physicochemical properties that the materials present in scales of nanometric size bring the attention of the researchers to their attributes. The nanoparticles used in this work were synthesized in order to have a double electric layer (EDL-MF) and by hydrothermal co-precipitation methodology it was possible to synthesize cobalt nanoparticles with core/shell structure, in which their core is covered by a layer of maguemite ($\Upsilon\text{-}Fe_2O_3$). The particles were subjected to a functionalization with citrate ion and separated in size in order to investigate their colloidal state. The physicochemical properties of the particles obtained by the synthesis of $CoFe_2O_4$-type nanoparticles were investigated by means of characterization techniques such as Diffractometry, X-Ray Diffraction, Transmission Electronic Microscopy (TEM), and Atomic Absorption Spectrometry (AAS) [2]. These particles were dispersed in a Deep Eutectic Solvent (DES) based on Choline and Urea, as it is shown to be a biocompatible and biodegradable solvent [3]. The particles were then lyophilized, which is the water withdrawal process from the samples, and the suspension of the particles dispersed in the DES was analyzed by the low angle X-ray scattering technique (SAXS).

[1] MUNIZ, R. P; Uso da força iônica para ajuste do estado coloidal de fluidos magnéticos aquosos. Trabalho de Conclusão de Curso em Ciências Naturais pela Universidade de Brasília. Brasília, 2019.
[2] BARRETO, C. C. K. Dispersão de Nanopartículas Magnéticas em Meios Complexos Biodegradáveis. Tese de Doutorado em Química em Co-tutela entre a Universidade de Brasília e a Université Paris IV. Paris, 2016.
[3] HAMAD, A. A; HAYYAN, M; ALSAADI, M. A; MASHIM, M. A; Potential applications of deep eutectic solventes in nanotechnology. Chemical Engeneering Journal, p. 551-567, 2015.

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P22

REMOVAL OF As(V) FROM AQUEOUS SOLUTIONS USING CORE@SHELL BIMAGNETIC NANOADSORBENTS

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Magnetic nanomaterials have emerged as potential adsorbents applied in toxic metals removal from aquatic medium. This study proposes the synthesis and characterization of core@shell magnetic nanoparticle aiming its application in the removal of pentavalent arsenic (As (V)) from aqueous solution. The nanoadsorbents were synthesized using a coprecipitation in alkaline medium followed by a surface treatment, leading to the final magnetic nanoparticle $CoFe_2O_4@\gamma\text{-}Fe_2O_3$. The adsorption capacity of the nanomaterial and influence of conditions of the medium were obtained using batch studies which evaluated the parameters pH, contact time, initial As(V) concentration, ionic strength (with NaCl), and the presence of phosphate and humic acid. After chemical adsorption, the nanoadsorbents loaded with As(V) were separated using a hand-held magnet and the final concentration of As (V) in the supernatant was determined by Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES). In addition, nanomaterials desorption and reuse tests were performed. The pH has been found to exert a major influence on the adsorption. The maximum adsorption was observed at pH = 2. The equilibrium adsorption was observed after 6 days, but within 24 hours, the As(V) removal exceeded more than 50% of the capacity. The presence of humic acid did not show significative influence in the As (V) adsorption. The NaCl exhibited a positive influence while the phosphate showed a negative influence in the As(V) adsorption. The maximum adsorption capacity using the Freundlich isotherm model was found 29.42 mg/g for pH = 4.5. Regeneration e reuse studies revealed that the nanoadsorbents can be recovered for reuse but with reduced adsorption capacity. These results indicate that prepared nanoadsorbents can be used as tool for As(V) removal from contaminated water.

[1] B. Monárrez-Corderoa, Mater. Res.19, 103 (2016)
[2] K. Rajendran, IJPRIF 8, 670-677 (2015)

P23

A DFT STUDY OF C18O2 HETEROFULLERENE ISOMERS

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In recent years heterofullerenes have been the focus of several studies, mostly theoretical, due to their possible use as gas sensors[2] and as hydrogen storage materials[3]. However, the vast majority deals with symmetric isomers of heterofullerenes containing 30 or more carbon atoms. A recent study[4] proposed AlC19 and BC19 as promising candidate materials for adsorption of H_2S and SO_2 toxic gases. The aim of this work is to investigate the relative stability, dipoles, HOMO-LUMO energy gaps and IR frequencies of six possible C18O2 bucky-bowl isomers.

The geometry of all proposed structures for C18O2 heterofullerene isomers were fully optimized, without any symmetry constraints, at the B3LYP/6-31G(d) level of theory using GAUSSIAN 09 software. Vibrational frequencies, dipole moment, HOMO, LUMO and total energies were calculated for this structures under the same conditions. All optimized structures were verified for the absence of negative frequencies to make sure they were true minima.

Assuming the most stable isomer as the energy zero, the six optimized structures showed relative energies varying from +32,3 to +101,6 kcal.mol^{-1}, HOMO/LUMO gaps between +31,3 and +59,5 kcal mol^{-1} and dipole moments between 0,15 and 2,54 D, suggesting that the isomers could be separated by chromatographic techniques if present in a synthetic product mixture. All isomers smallest vibrational frequencies were above 100 cm^{-1}, confirming they are true minima of stable molecules[1]. Some of the frequencies higher than 1000 cm^{-1} could be used to characterize the species by IR spectroscopy. We conclude that the calculated properties can be used as a guide for experimentalists in separating and characterizing the C18O2 heterofullerene bucky-bowls isomers. Future studies of changes in HOMO/LUMO gaps with adsorbed gases could access their possible use as gas sensors.

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[1] R. Hoffmann , P. Schleyer and H. Schaefer, Angewandte Chemie International Edition, 47: 7164-7167 (2008)
[2] M. Baei, K. Tavakoli, S. Hashemian & P. Torabi, Fullerenes, Nanotubes and Carbon Nanostructures, 23:2, 153-157 (2015)
[3] S. Amiri, M. Koohi and B. Mirza, *J. Phys. Org. Chem.*, 29: 514– 522. (2016)
[4] F. Molani and M. Askari, *J. of Structural Chem.*, 58:4, 657-666 (2017)
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P24

SINGLET EXCITON DIFFUSION LENGTH IN BENZODIINDOLIZINES DERIVATIVES

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In the last decades, researchers have worked on the improvement of organic electronic devices. In particular, in the field of organic solar cells, the study of exciton diffusion is of great relevance since this process influences device efficiency considerably. Exciton behavior is highly dependent on both the molecule's electronic properties as well as its crystalline arrangement. Recently, a set of seven N-heteroaromatic[1] compounds has been synthesized forming molecular crystals. These systems have shown promising properties for applications in organic electronics, which calls for further theoretical investigation regarding exciton diffusion. Here, we use density functional theory (DFT) to obtain the electronic proprieties of these seven molecules. In addition, combining absorption and emission spectrum simulations with the corresponding crystalline structures allows us to estimate singlet exciton diffusion length[2] in these compounds. We show that these compounds present large exciton diffusion lengths that are dependent on crystalline axes. Our results provide theoretical insight into the behavior of excitons in this set of organic molecular crystals.

[1] GRANGER, Devin B., et al. Synthesis and Electrical Properties of Derivatives of 1, 4-bis (trialkylsilylethynyl) benzo [2, 3-b: 5, 6-b′] diindolizines. Organic letters (2016).
[2] SOUSA, Leonardo et al. Fast Predictions of Exciton Diffusion Length in Organic Materials. Journal of Materials Chemistry C (2019).

P25

Understanding the importance of Chlorophylls, Carotenoids, and Xanthophylls in photosynthesis by the Förster Resonance Energy Transfer Study

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Photosynthesis is the most important solar energy conversion process in nature. Initially, its functioning relies on the capacity of light absorption of organic compounds such as carotenoids, chlorophyll, pheophytins, among other molecules. One may say that the absorption of light generates excitons, which are bound electron-hole pairs that carry energy. These quasiparticles diffuse through the system, eventually reaching reaction centers where the charge separation process may occur[1]. The efficiency of the diffusion process is contingent on the spectroscopic properties of the involved molecules, as well as, on the morphology of the whole system. The complex interplay between these features requires further studies on these steps of the photosynthetic process. In this work, a combination of quantum chemical calculations and spectroscopic simulations[2] is employed to understand the behavior of excitons in photosynthetic systems composed of different molecular species. We were able to calculate the efficiency of the exciton diffusion process in several molecules, as well as, the characteristic time for these energy transfers. Finally, we also present estimates of exciton diffusion length for the set of molecules. This work provides insight into the working of photosynthetic systems that may also be useful for technological applications like organic photovoltaic devices.

[1] Nelson, N., Ben-Shem, A., Nature Reviews Molecular Cell Biology, 5, 971–982 (2004)
[2] Sousa, L. et al., Phys. Chem. Chem. Phys., 21, 1711-1716 (2019)

P26

A COMPARATIVE STUDY OF PROTOCOLS FOR EXCITON DIFFUSION LENGTH ESTIMATION

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Exciton diffusion is one of the main processes present in organic optoelectronic devices such as organic light emitting diodes (OLEDs) and organic solar cells (OSCs) [1,2]. This is the case because of the large exciton binding energy resulting from low dielectric constants usually observed in organic materials. Given the large amount of organic compounds available, computational protocols that are able to predict exciton diffusion lengths are a necessary tool to guide the rational design of devices. Recently, a computational procedure that relies on the simulation of absorption and emission spectra has been proposed [3]. In this procedure, quantum chemical calculations are combined with an analytical model to produce estimates of exciton diffusion length. In this work, we reproduced the cited protocol using the nuclear ensemble method, but now, controlling the geometries' input. The obtained results were compared with simulations generated previously. Our results show that even with a small variation on the Förster radius a more significant discrepancy is observed in the diffusion length. This investigation impacts the development of strategies for the rational design of devices since it allows reuse of the geometries sorted for later simulations.

[1] B. Kippelen, J. L. Bredas, Energy Environ. Sci. v. 2, p. 251-261 (2009)
[2] L. E. Sousa et al, J. Mater. Chem. C, v. 7, p. 4066-4071 (2019)
[3] L. E. Sousa, P. H. de Oliveira Neto, Phys. Chem. Chem. Phys., v. 21, p. 1711-1716 (2019)

P27

POLYOL SINTHESIS CONDITIONS FOR COBALT FERRITE NANO-OBJECTS AND FERROFLUID ELABORATION

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Magnetic nanoparticles (MNPs) have been the subject of intense research for several years, due to their striking different physicochemical properties and their potential for practical applications. However, some of these properties such as, cationic distribution, size, polydispersity, magnetic properties can be strongly changed depending adopted synthesis procedures. Therefore, in the present study we want to investigate a new synthesis route that would allow the production of morphologically homogeneous magnetic nanoparticles, chemically stable and with very low size dispersion. Through the polyol route, cobalt (II) and iron (III) chlorides were used as precursors in a mixture of the solvents Dietylene glycol (DEG) and Triethanolamine (TEA) in different proportions (1:0 and 1:1), seeking the formation of cobalt ferrites. In addition to the proportion of polyols, other parameters were investigated, such as reaction time and presence of a basic reactant. The performed synthesis pursued the formation of monocore magnetic nanoparticles, and we added TEA aiming to form multicore nano-objects. All the synthesis process has been performed with different duration and the obtained product has been dried and characterized by X-ray diffraction, Transmission Electron Microscopy (TEM) and Atomic Absorption Spectroscopy (AAS). The results show that only 1:0 ratio synthesis yielded magnetic nanoparticles, proving very small nanoparticles, almost monodisperse in size and with good crystallinity. The change in reaction time led to a slight variation in the mean diameter of the MNPs obtained and the base was proved to be essential on the formation of the ferrites MNPs. Magnetic Fluids will be elaborated with this MNPs and characterized magnetically.

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USING RAMAN SPECTROSCOPY FOR IDENTIFICATION OF THREE MICROALGAE SPECIES

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Microalgae are photosynthetic organisms rich in lipids, proteins and pigments [1]. These biomolecules are important to the cosmetic, food, pharmaceutical, etc. In particular, the potential of microalgae as a commercial source of pigments was widely recognized and studied [2]. In this work, we propose to use Raman spectroscopy (ER) combined with multivariate analysis to study three species of microalgae (Chlamydomonas sp. (CA), Chlorella s. (CO) and Nannochloropsis o. (NN)) to determine the relative content between carotenoids and chlorophyll in these species. Usually, when performed with the laser line tuned around 520 nm, the algal Raman spectrum were dominated by three intense bands at ~ 1005, 1157 and 1527 cm^{-1}. These bands were attributed to the stretching vibrations $\nu(\mathrm{C}-\mathrm{CH}_3)$, $\nu(\mathrm{C}-\mathrm{C})$ e $\nu(\mathrm{C}=\mathrm{C})$ associated to carotenoids. However, when obtained with a laser line tuned close to the Soret absorption band, the Raman spectrum of the same sample shows new characteristic bands of the porphyrin molecule in the region of 1200 - 1400 and 1550 - 1700 cm^{-1} , these new bands can be associated with the chlorophyll Raman signal [3]. Raman spectra obtained for the three microalgae species have very similar characteristics. Thus, in order to determine whether Raman spectra can be used to distinguish different species of algae, principal component analysis (PCA) tools were employed. The result of this analysis showed variances greater than 98%. In addition, in order to verify the relative content between carotenoids and chlorophyll present in algae species, the ratio between the integrated intensities of the typical vibrational modes of carotenoids and chlorophyll were obtained. This study show that the carotenoid content is lower in CO microalgae and higher in NN microalgae when compared to CA microalgae. The Raman results were confirmed by the UV / VIS, technique used often for this purpose.

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References:

[1] Borowitzka, M., *et al*. Elsevier Applied Science, 1988. 371-381.
[2] Shixuan, H., *et al*. Molecular Spectroscopy 190 (2018): 417-422.
[3] Feiler, Ute, *et al*. Journal of Raman spectroscopy (1994): 365-370.

P29

ENERGETIC AND VIBRATIONAL DISORDERS ON EXCITON DYNAMICS IN ORGANIC THIN FILMS

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The understanding of exciton dynamics is of fundamental importance in the field of organic semiconductors. Many aspects may affect the diffusion and recombination of excitons in organic materials, among which the absorption and emission spectra of the molecules, as well as, morphological and energetic disorders [1]. Disorder effects on exciton diffusion have been studied, usually assuming a particular shape for the density of states. In this sense, a method that takes into consideration the individual properties of particular molecules is required. In this work, we study the effects of disorder produced by molecular vibrations and different energies in each site on singlet exciton diffusion in aluminum tris-(8-hydroxyquinoline) (AlQ3) [2] molecules. By means of Density Functional Theory (DFT), the absorption and emission spectra of several molecular conformations that result from vibrations are computed. These features are used to predict changes in the dynamic of excitons in this material by producing estimates of exciton transfer rates, which serve as input to Kinetic Monte Carlo simulations. These simulations, in its turn, allow us to calculate exciton diffusion length and decay time [3]. Comparisons are made with similar simulations performed disregarding both effects. Our results shed light on the role played by vibrations and energetic disorder in exciton diffusion in a typical organic material.

[1] C. Madigan, V. Bulovic, Phys. Rev. Lett. 96, 046404 (2006)
[2] H. Li et al., Materials Science and Engineering B100, 40-46 (2003)
[3] L. E. Sousa et al., J. Chem. Phys., 148, 204101 (2018)

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THE EFFECTS OF VIBRATIONAL DISORDER IN SINGLET EXCITON DIFFUSION IN ORGANIC COMPOUNDS

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Organic photovoltaic cells (OPV) are widely studied and show promise as potential successors to conventional silicon-based photovoltaic cells[1]. In these devices, exciton diffusion plays an essential role, since excitons must reach donor-acceptor interfaces for charge transfer to take place. Singlet exciton diffusion results from a non-radiative mechanism known as the Förster resonance energy transfer. The efficiency of this process is governed by the interplay between the spectroscopic properties of the chosen materials and disorder effects [2]. Thus, it is paramount to understand how these two quantities may affects the exciton diffusion in general, and also the specifics of how different individual molecules respond to vibrational disorder. Here, we perform spectra simulations of several molecular compounds of interest in the field of organic electronics [3] under disorder effects. Our results show different responses to vibrational disorder, where an enhancement or hindering of the Förster transfer rate may occur. We were able to identify when the vibrational disorder will favor the exciton dynamics by a statistical analysis of the nuclear ensemble. The understanding of this mechanism in organic materials will allow for the enlightened selection of more appropriate donor and acceptor compounds for each device's purposes.

[1] B. Kippelen, J. L. Brédas, Energy Environ. Sci. 2, 251-261 (2009)
[2] P. Peumans et al., J. Appl. Phys., 93, 3693 (2003)
[3] L. E. Sousa et al, J. Mater. Chem. C, 7,4066-4071 (2019)

P31

INVESTIGATION OF PHOTO-INDUCED ELECTRICAL RESPONSE UNDER GAS INCIDENCE IN SnO_2: 1%at Er^{3+} BASED THIN FILM SAMPLES

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Tin oxide (SnO_2) is a *n-type* oxide semiconductor with many applications, such as gas sensors, due to its sensitivity to many gases, including reducing and toxic gases (such as acetone, carbon monoxide and others) [1]. The principle of gas sensors operation is related to changes in conductance when detecting a particular gas, which can be improved when SnO_2 is in the form of nanoparticles (increases surface area), doped or mixed with other metal oxides, that depends on type of gas and operating conditions. This work presents results of electrical measurements (photo-induced current decay) on isolated Er-doped SnO_2 thin films (particle size about 10nm) and combined with GaAs in the GaAs/SnO_2:Er heterojunction. SnO_2 is deposited by resistive evaporation technique, where the powder for evaporation is obtained by the sol-gel route, as recently reported [2]. Measurements were performed after excitation with distinct light sources: He-Ne laser (628nm) and InGaN LED (450nm), under influence of atmosphere rich in CO_2 or O_2. Electrical conductivity of SnO_2:1at%Er^{3+} sample, annealed at 1000ºC, changed significantly when exposed to these gases. Excitation with the LED at room temperature leads to decay rate (calculated from the maximum current) of 8.2% for O_2 and 21.6% for CO_2, for 50s of stabilization time in the sample current. Although these light energies are lower than the SnO_2 bandgap, they have high influence on excitation, ionizing efficiently intrabandgap states. The CO_2 gas induces electron capture from the sample even in the dark, which is enhanced under light irradiance. GaAs/SnO_2 heterostruture showed smaller stabilization time when compared to SnO_2 samples. This effect may be related to the interface between SnO_2 and GaAs films, which have many defects, leading to electron trapping at the interface.

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[1] A. Dey. Mater. Sci. & Eng. B 229, 206 (2018)
[2] D. H. O. Machado et. al., Mater. Res. Bull. 120, 110585 (2019)

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OLIGOMER SIZE EFFECTS ON EXCITON DIFFUSION LENGTH

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The study of exciton dynamics is essential since it constitutes a key aspect concerning the efficiency of organic optoelectronic devices [1]. Conjugated polymers have been widely used in such applications for their charge and energy transport properties. In this sense, it is necessary to understand the mechanism behind exciton transfer in this class of materials. Previous studies have been able to provide estimates of exciton lifetime and diffusion length for small molecules by means of spectrum simulations [2]. However, the direct application of similar procedures for long polymeric chains would be computationally impracticable. In that matter, alternative treatments are required. In this work, we perform spectrum simulations for poly(p-phenylene vinylene) and polythiophene by analyzing the evolution of electronic properties with oligomer sizes. In conjunction with the Kuhn model [3], results allow us to determine optical excitation energies in the polymeric limit. Furthermore, we investigate the dependence of interchain exciton diffusion efficiency on oligomer size. Our results demonstrate how to well describe optical properties in the polymeric limit and its effects on interchain exciton diffusion. This study may be useful in the development of more sophisticated optoelectronic devices that use conjugated polymers as its active materials.

[1] Kippelen, B. and Brédas, J.-L., Energy & Environmental Science 2, 251-261 (2009).
[2] Sousa, L. et al., Journal of Materials Chemistry C 7, 4066-4071 (2019).
[3] Gierschner, J., Cornil, J., and Egelhaaf, H.-J., Advanced Materials 19, 173-191 (2007).

P33

DESIGNING TUMOR SPHEROIDS TECHNOLOGIES FOR 3D IN VITRO BRAIN CANCER MODEL FOR NANOMEDICINE SCREENING

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In glioblastoma multiforme (GBM), maximum surgical resection, radiotherapy, and adjuvant temozolomide is the golden standard of care, yet it could only provide a median survival around 15 months [1]. Medulloblastoma (MB) is made up of least four clinically and molecularly distinct types of tumours [2]. Tumor spheroid represents highly suitable 3D organoid-like framework elucidating the intra and inter cellular signaling of cancer, like that formed in physiological niche [3]. The present study investigates the spheroid formation in 3D cultures and the gene expression profile of signaling pathway the epidermal growth factor (EGF) in GBM and MB lines after treatment with photodynamic therapy (PDT). The GBM cells lines (U343 and U87MG) and MB (UW473) were cultured (DMEM, 4-5 days, at 37°C, 5% CO_2/95%) and treated with the chloroaluminium phthalocyanine-containing nanocarrier subjected to treatment with monochromatic laser light. The combination of brain tumors and studies involving PDT at the molecular level allowed the discovery of genes that participate in the regulation of the gene expression of other signaling pathways such as RTK/Ras/PI3-K and AKT/MAPK. Such pathways are responsible for increased cell proliferation, survival and resistance to apoptosis, loss of adhesion/migration that may reveal a high degree of tumor invasiveness. The diagnostic and prognostic role of spheroids rearrangements within biomaterials or microfluidic channel is indicative of patient management; particularly for the decision of targeted therapy. These findings confirm that the engineering of nanocarriers associated with PDT procedures led to the hypoexpression of the genes that are directly involved in the EGF tumor process. Such findings contribute to the development of advanced protocols that may aid in the in vivo assays available for clinical oncology.

[1] I. Elmaci, A. Bilir, A. Ozpinar, M. A. Altinoz, Tissue Cell 59 (2019)
[2] D. P. Ivanov, T. L. Parker, D. A. Walker, C. Alexander, et al. J. Biotechnol. 205 (2015)
[3] T. Rodrigues, B. Kundu, J. Silva-Correia, S. C. Kundu, et al, Pharmacol Ther. 184 (2018)

P34

IMPROVEMENTS OF DLVO THEORY APPLIED TO MAGNETIC NANOPARTICLE INTERACTION IN FERROFLUIDS

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A ferrofluid is a colloidal dispersion of magnetic nanoparticles in a liquid, with technological and biomedical applications related to its strong response to magnetic field while keeping its fluid properties [1]. Ferrofluids are frequently described through an extended DLVO theory [2] which adds a magnetic dipolar interaction to the van der Waals (vdW) and electric double layer (EDL) forces. However, the traditional vdW and the EDL interaction energy expressions present serious limitations. The vdW energy diverges as the distance between the surfaces of two nanoparticles approaches zero, thus a minimum distance cutoff must be specified in order to perform calculation of average properties. The EDL energy, in turn, has alternative models that are valid to surface-surface distances that are either very small or very large compared to the diameters of the interacting nanoparticles. Improvements on the vdW and EDL interaction models have been suggested, aimed at solving these limitations. Here, we analyze the influence of some of these modifications on the pair interaction energy curves for magnetic nanoparticles of ferrofluids. For the vdW interaction, we analyze the critical distance and maximum wavenumber approaches [3] while, for the EDL interaction, we test the an application of so-called ray theory [4] which allows us to write down an energy expression which is valid for all separation distances. By means of this interaction model, we expect to reduce parameter arbitrariness and improve the accuracy of the results of future computer simulations of ferrofluids.

[1] ROSENSWEIG, R. E. Ferrohydrodynamics. Mineola, Nova York: Dover, 1997.
[2] RUSSEL, W. B.; SAVILLE, D. A.; SCHOWALTER, W. R. Colloidal dispersion. Cambridge: Cambridge University Press, 1989.
[3] WHITE, L. R. van der waals interaction energy and disjoining pressure at small separation. Journal of Colloid and Interface Science, v. 343, n. 1, p. 338–343, 2010.
[4] SCHNITZER, O.; MOROZOV, M. A generalized derjaguin approximation for electrical-double-layer interactions at arbitrary separations. The Journal of Chemical Physics, v. 142, n. 244102, 2015.

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SERS ACTIVE SUBSTRATES MADE BY PHOTOCATALYTIC DEPOSITION OF Ag NANOPARTICLES

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Layer-by-layer assembled photocatalysts films of TiO_2 nanoparticles (TiO_2NP) combined with either sulfonated polystyrene (PSS) or graphene oxide (GO) are employed for the photodeposition of Ag nanoparticles and subsequently used in surface-enhanced Raman scattering. Both photocalysts films, TiO_2NP/PSS and TiO_2NP/GO, are capable of driving the formation of AgNP when kept immersed into $AgNO_3$ diluted solution under UV irradiation (254 nm). The rate constants of AgNP formation, determined by UV-vis spectroscopy, are basically the same at both films. Nonetheless, scanning electron microscopy reveals that in the TiO_2NP/PSS film, the photodeposited AgNP are larger and isolated, while in the TiO_2NP/GO film, they are smaller and highly inter-connected. The Raman spectrum of rhodamine B (model probe) is enhanced at both films; however, the enhancement is much higher at the TiO_2NP/GO film, because GO is a suitable anchoring harbor for interconnected AgNP and also quenches the fluorescence emission of rhodamine B, something that PSS is unable to do. The enhancement is even more pronounced when samples are excited at 633 nm, because of the resonant condition with the rhodamine B absorption.

[1] I. A. Costa et al., J. Phys. Chem. C 122, 24110 (2018).
[2] B. N. Nunes et al., J. Photochem. Photobiol. C: Photochem. Rev. 32, 1 (2017).

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Molecular Dynamics of Pure Liquids - Octane, Nonane and Benzonitrile Benchmark of the OPLS Force Field

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There is great interest in obtaining thermodynamics excess properties for multi-component mixtures of liquids by molecular simulations, not only to obtain accurate properties such as densities, heat of vaporization, among others, but to also to understand the structural changes as a function of temperature and composition [1]. For such purpose an accurate force field and simulation protocol for pure liquids in broad temperature range is needed before applying the model to mixtures.

In this study the heat of vaporization, heat capacity, thermal expansion coefficient and densities were obtained for octane, nonane and benzonitrile with the purpose of evaluating the performance of OPLS-AA [2] force field for the need of future modifications required to simulate mixtures. TINKER 8.4 software [3] was used for all 1 atm NPT 4ns simulations on periodic boundary cubic boxes and 2fs interval r-Respa integrator based on Beeman [4].

Simulated properties were compared with accurate experimental data [1] at temperatures ranging from 283K to 363K. Heat capacities have poor accuracy with relative errors larger than 100%. Relative average errors of 44,7%, 42,1% and -1,5% were obtained for thermal expansion coefficients of octane, nonane and benzonitrile respectively. A fairly good accuracy was obtained for densities in general for all molecules underestimated with relative errors lower than 3.5%, however super-estimated thermal coefficient for alkanes put in evidence the weakness of the force field to correctly model temperature effects on density behavior. Also, all simulated heat of vaporization were underestimated by up to 14%. These findings suggest that attraction forces were underestimated and original OPLS-AA van der Waals parameters for alkanes need to be modified. Parameters for benzonitrile show better accuracy and correct temperature behavior, probably due to the fact that it is a more rigid molecule with dominant Coulomb forces interactions.

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[1] Lei, Y.; Chen, Z.; An, X.; Huang, M.; Shen, W. Measurements of Density and Heat Capacity for Binary Mixtures {x Benzonitrile + (1 -x) (Octane or Nonane)}. J. Chem. Eng. Data, 55, 4154–4161 (2010).
[2] Jorgensen, W. L.; Julian D. S. M.; Tirado-Rives. Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids. J. Am. Chem. Soc. 118, 45, 11225-11236 (1996).
[3] Rackers J. A., Wang Z., Lu C., Laury M. L., Lagardere L., Schnieders M. J., Piquemal J., Ren P., Ponder J. W. Tinker 8: Software Tools for Molecular Design. J. Chem. Theory Comput., 14, 5273−5289 (2018).
[4] D. Beeman, Some Multistep Methods for Use in Molecular Dynamics Calculations, J. Comput. Phys., 20, 130-139 (1976).

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IMPACT OF TUNING THE LONG RANGE PARAMETER ON EXCITON DIFFUSION LENGTH PREDICTIONS IN ORGANIC SYSTEMS

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Theoretical descriptions of exciton dynamics are essential for the rational design of new organic optoelectronic materials[1]. Time-Dependent Density Functional Theory (TD-DFT) is widely employed in the study of electronic properties such as optical excitation energies. Such properties have been used to predict important features that are key to the design of efficient devices. One such feature is the exciton diffusion length, which is the typical distance excitons are able to travel before recombining. It has been shown that this quantity may be estimated by means of spectrum simulations that make use of TD-DFT[2]. In this sense, techniques that are able to improve the reliability of such methods are of paramount importance. In this work, we investigate the impact of tuning the range-splitting parameter present in range-separated hybrid functionals on estimations of singlet exciton diffusion lengths for a set of organic molecules of interest to the field of organic electronics. Results are compared to experimental data indicating that the procedure shown here greatly improves the reliability of predictions, constituting an important tool for the description of exciton dynamics in organic materials.

[1] Kippelen, B. And Bredas, J. -L, Energy & Environmental Science vol 2, 251-261 (2009);
[2] L. E. Sousa et al, J. Mater. Chem. C, 7,4066-4071 (2019).

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Investigation of the magnetic properties of $CoFe_2O_4$@γ-Fe_2O_3 core/shell nanoparticles

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We prepare, by the coprecipitation method, core/shell (CS) nanoparticles (NPs) of different sizes of $CoFe_2O_4$ ferrite core surrounded by a (γ-Fe_2O_3) (maghemite) shell ($CoFe_2O_4$@γ-Fe_2O_3).

The microstructural properties of these NPs are investigated by XRD and TEM experiments. The mean size diameter, determined by XRD measurements, ranges from 4,5 to 11 nm. Previous investigations of core/shell NPs prepared by the same method and with same size demonstrated that the inner region has a well-ordered ferrimagnetic structure, surrounded by a surface small layer of spins randomly frozen at low temperatures[1]. This disordered surface contribution is evidenced by under-field Mössbauer spectroscopy measurements[2], showing a progressive spin alignment under field along the ferrite core.

In this work we investigated the influence of the size diameter on the magnetic properties and in particular on the exchange bias (EB) effect. Mössbauer spectra recorded 12K under intense magnetic field (8T) shown the presence of the surface spin disorder, as observed previously. This disorder is clearly more evident for NPs of smallest size diameter. The EB field H_{ex}, measured at 5K after cooling under a field of 3 kOe, is present for all the samples and it increases as the size particle of the NPs decreases (11 nm; H_{ex}15 Oe, 5,4 nm; H_{ex}105 Oe ; 4,5 nm; H_{ex} 155 Oe). For the smallest particle size (4,5 nm) we investigated the interparticle interaction role of magetic interations on the blocking and exchange bias properties. The interparticle interaction is then tuned by the NP volume fractions, ranging here between 0.4% and 18% using the osmotic stress technique[3] and compared to the powder sample.

The Hex obtained for the samples investigated here confirms the role of interparticle interations as seen in[4].

[1] Aquino R, Depeyrot J, Sousa MH, Tourinho FA, Dubois E, Perzynski R. Magnetization temperature dependence and freezing of surface spins in magnetic fluids based on ferrite nanoparticles. *Phys Rev B - Condens Matter Mater Phys*. 2005;72(18):1-10. doi:10.1103/PhysRevB.72.184435

[2] Sousa EC, Rechenberg HR, Depeyrot J, et al. In-field Mossbauer study of disordered surface spins in core/shell ferrite nanoparticles. *J Appl Phys*. 2009;106(9):1-7. doi:10.1063/1.3245326

[3] Cousin F, Dubois E, Cabuil V. Tuning the interactions of a magnetic colloidal suspension. *Phys Rev E - Stat Physics, Plasmas, Fluids, Relat Interdiscip Top*. 2003;68(2):9. doi:10.1103/PhysRevE.68.021405

[4] Silva FG, Raikher YL, Depeyrot J, et al. The role of magnetic interactions in exchange bias properties of MnFe 2 O 4 @ γ -Fe 2 O 3 core/shell nanoparticles. *J Phys D Appl Phys*. 2013;46(28):285003. doi:10.1088/0022-3727/46/28/285003

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Exploring Mg and Bi as catalysts for wurzite InP nanowire growth

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Semiconductor nanowires (NWs) are currently under intense investigation, both as basic science, to understand the nanostructure formation dynamics, and for technological applications in areas such as optoelectronics andenergy harvesting, among many others. Au catalysts have been widely explored in semiconductor nanowiresynthesis; however, some characteristics of this type of synthesis limit the potential nanowire applications. Inthis work, we explore Mg and Bi as catalysts for InP nanowire growth. Mg and Bi have been used as a dopantin InP thin films [1,2]. We explore the possibility of catalyst consumption during growth, creating InP: Mg and InP: Bi NWs. For these reasons, this material is a good alternative to the use of Au as a catalyst. In this work,the nanowires have been grown by Chemical Beam Epitaxy. Scanning electron microscopy provides nanowire shape statistics and Energy-dispersive X-ray spectroscopy and transmission electron microscopy were used toinvestigate nanowire chemical and structural properties, respectively.

By varying the temperature we observe thin and long Bi and Mg catalyzed InP nanowires. For lower temperatures, we do not observe the metallic catalyst on the NW apex, which suggests it is consumed during growth. For higher temperatures, we observe a particle on the NW apex (the particle size varies with the temperature) and oscillations along the nanowire length, consistent with Vapor-Liquid-Solid growth model [3]. It is under investigation if Mg and Bi are incorporated only as impurity in InP or if it also forms clusters. TEM shows that the nanowires present a wurtzite lattice structure. The NW density for each population varies with the In precursor flow and growth temperature.

Our results suggest an In-assisted growth regime, with Mg and Bi nanoparticles participating in the process. Analyzing the composition and morphology of the apex nanowires, grown at higher temperatures, we conclude they are indeed grown by the VLS method. The optical properties are currently under investigation.

[1] Blaauw, C. et al. Characterization of Mg-doped InP grown by MOCVD using a bis(methylcyclopentadienyl)magnesium dopant source. J. Electron. Mater. 18, 567-572 (1989).
[2] Wu, X. et al. Anomalous photoluminescence in $InP_{1-x}Bi_x$. Sci. Rep. 6, 27867 (2016).
[3] Oliveira, D. S., Tizei, L. H. G., Ugarte, D. and Cotta, M. A. Spontaneous Periodic Diameter Oscillations in InP Nanowires: The Role of Interface Instabilities. Nano Lett. 13, 9-13 (2013).
[4] Oliveira, D. S. et al. Different growth regimes in InP nanowire growth mediated by Ag nanoparticles.Nanotechnology 28, 505604 (2017).

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MORPHOLOGY-DESIGN OF ZnO NANOSTRUCTURES AND ITS CORRELATION WITH THE STRUCTURAL, VIBRATIONAL AND OPTICAL PROPERTIES

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Nanostructured systems show novel electrical, optical and chemical properties, which are notoriously different from their bulk counterpart. Among the nanostructured systems, zinc oxide (ZnO) has been of interest due to the wide band gap energy (Eg~3.4 eV), large exciton energy at room temperature (~60 meV) and good electrical properties which could be used in a wide range of applications, such as sensors, solar cells and photodegradation of organic pollutants [1-3]. Several approaches have been developed to prepare ZnO powders, such as sol-gel, microemulsion, thermal decomposition of organic precursor, spray pyrolysis, electrodeposition, ultrasonic, microwave-assisted techniques, chemical vapor deposition, hydrothermal and precipitation methods, obtaining different properties, morphologies and sizes.
In this work, we study the nucleation and growth mechanism of rod-, needle-, nut- and doughnut-like ZnO morphologies with distinct particle sizes and surface areas; and the influence of physical-chemical parameters—such as the solvent and the pH of the solution—on the morphology, as well as the structural and optical properties. We found a clear correlation between the growth rate along the c-axis and surface defects. Our results suggest that the needle- and rod-like morphologies are formed due to the crystal growth orientation along the c-axis and the occurrence of crystalline defects, such as oxygen vacancies and interstitial Zn2+ located at the surface, whereas nuts and doughnuts are formed due to growth along all crystalline planes except those related to growth along the c-axis. In addition, the structure morphology changes systematically with temperature, driven by the ZnO crystal planes anisotropy and obeying the crystal growth theory. As a result, ZnO in needle-, rod-, nut-, and doughnut-like shapes are easily fabricated in the aqueous solution with a high crystallinity and uniformity.

Based on the experimental results, growth mechanisms for the formation of ZnO structures were proposed. We believe this synthesis method will be readily adopted in realizing different shapes for various materials and for specific applications.

Keywords: ZnO structures, ZnO synthesis, morphology control, shape control, growth mechanisms.

[1].Teke, A. et al. Physical Review B 2004, 70 (19), 195207.
[2].Zhang et al. Journal of Catalysis 2015, 331, 57-62.
[3].Montero-Muñoz, M. et al. Applied Surface Science 2018, 448, 646-654.

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ATOMIC-LEVEL AND ELECTRONIC STRUCTURE INSIGHT OF Co^{2+}-DOPED ZnO NANOCRYSTALS

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Intentional transition-metal (TM) doping of Zinc Oxide (ZnO)─with Fe, Co, Ni and/or other TM─has been motivated by the possibility of obtaining ferromagnetism at room temperature which finds a wide application in spintronics, magnetic switches, magnetic sensors, and many others[1,2]. The results are very controversial and depend to a great extent on the synthesis conditions, which calls for a critical and detailed analysis starting from the structural characterization.

In this work, we have synthesized and performed a detailed structural and electronic study of pure and Co-doped ZnO NCs obtained via the sol-gel method. The nanocrystals were characterized by conventional macroscopic techniques, such as X-ray Diffraction (XRD), High-Resolution Transmission Microscopy (HRTEM), X-ray Photoelectron Spectroscopy (XPS) and element-specific advanced tools, such as X-ray Absorption Near-Edge Spectroscopy (XANES) and X-ray Absorption Fine Structure (XAFS). The XRD and HRTEM data analysis indicate the formation of pure and doped ZnO NCs in the wurtzite structure, with circular- and elliptical-like shapes─with changes in the structural parameters with the dopant content. The Zn K-edge EXAFS results revealed a good similarity between the synthesized ZnO NCs and bulk ZnO compound. The peak intensity relative to Zn–Zn contributions suggests the presence of zinc vacancies in our samples. In addition, the experimental EXAFS signal measured at the Co K-edge showed features consistent with those ones showed by the Zn K-edge of pure ZnO NCs providing clear evidence that Co ions are in similar environment as Zn ions in pure ZnO NCs. The higher intensity of XANES pre-edge peak in comparison to that of reference samples corroborates that the Co ions occupy tetrahedral sites in the wurtzite lattice. Besides, XPS and XANES results indicate that Co assume predominantly the 2+ valence state and confirms the occupation of tetrahedral sites.

[1] J. Theerthagiri, S. Sunitha, R. A. Senthil, P. Nithyadharseni, A. Madankumar, P. Arunachalam, & H. S. Kim. Nanotechnology 30, 392001 (2019)
[2] H. Hong. Magnetic Oxide Semiconductors. In: Xu Y., Awschalom D., Nitta J. (eds) Handbook of Spintronics. Springer, Dordrecht (2016)

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DIRECT REALIZATION OF MICROSTRUCTURE CHANGES IN SOME METAL OXIDE NANOSTRUCTURES BY RAMAN SPECTROSCOPY AND ELECTRON MICROSCOPY

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The observations of microstructure variation or structural transformation along with its light absorption properties are essential in wide band gap semiconductor nanomaterials such as TiO_2, SnO_2, ZnO etc. In this context, the spectroscopy and microscopy measurements are very crucial and important to realize these microstructural changes directly for a better understanding of the nanostructures. Transmission electron microscopy (TEM) is a powerful tool to directly visualize such microstructural changes in metal oxide nanomaterials whereas Raman spectroscopy is an important sensitive tool to detect molecular electronic structure and vibration levels in nanomaterials. In this work undoped TiO_2, undoped SnO_2, different concentration of Co and Ag doped TiO_2 nanoparticles; reduced graphene oxide (RGO) decorated Ag doped TiO_2 nanocomposites; and Co doped SnO_2 nanomaterials were prepared by cost effective sol-gel method. The influence of low concentration Co doping in TiO_2 nanoparticles and Co doping in SnO_2 nanoparticles on their structural transition, localized microstructure variation and optical properties were deeply studied by confocal Raman spectroscopy. The laser power dependent Raman spectra in increasing and decreasing order of the laser power were recorded in different spot of the samples in Co doped TiO_2 nanoparticles and Co doped SnO_2 nanoparticles. In both set of the samples the microstructure changes as a function of irradiating laser power were observed very clearly [1]. In Co doped TiO_2 samples the structural transformation were irreversible whereas the Co doped SnO_2 sample have shown reversible behaviour with improved localized structural properties. The silver doped TiO_2 and RGO decorated Ag doped TiO_2 nanostructures were rigorously probed by TEM to observe the phase transformation in anatase TiO_2 nanoparticles [2]. These results suggest that the semiconducting materials or phase changing materials which have different unstable polymorphs can lead to similar structural transformation either by high dopant concentration with even low power Raman measurements or low doping concentration at moderate or high laser power measurements.

[1] L. K. Gaur et al., J. Alloys Comp., 780 (2019) 25-34.
[2] M. C. Mathpal et al., Phys. Chem. Chem. Phys., 2014 (16) 23874-23883.

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REMOVAL OF LEAD FROM AQUEOUS SOLUTIONS BY CYSTEINE-COATED MAGNETIC NANOPARTICLES

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Lead is one of the most dangerous heavy metals and occupies the second place in the substance priority list compiled by the Agency for Toxic Substances and Disease Registry. This toxic metal causes a lot of damages in human health and environment. The water and soil remediation due to Pb(II) contamination remains a challenge [1]. Among the forms of metal segregation in mineral and industrial waters, the most common used methods are chemical fixation, ion exchange, membrane filtration, electrolytic methods, osmosis reversion, solvent extraction and adsorption by activated charcoal [2]. In this work, we investigated the removal of lead from aqueous solutions using innovative magnetic nanoadsorbents based on core@shell ferrite nanoparticles (NP) modified with L-cysteine (Cys). The nanoadsorbents were elaborated using the wet coprecipitation method in alkaline medium followed by a surface treatment with $Fe(NO_3)_3$. Controlling the pH of the synthesis medium, samples composed of nanoparticles of two different mean sizes were produced. The surface modification was carried out by mixing the NP and Cys in a solution methanol/water [3]. X-rays diffraction and TEM experiments were used to determine the crystalline mean size of the nanoparticles and FTIR measurements was used to evidence the surface modification. The influence of contact time, pH and initial Pb(II) concentration were evaluated from batch studies using 1.33 g/L of the nanoadsorbent. The Langmuir and Freundlich models were applied in order to evaluate the maximum adsorption capacity and the characteristic of the adsorption process. The kinetics data from the batch studies were analyzed with pseudo-first order, pseudo second-order and intraparticle diffusion models to evaluate the equilibrium time and kinetic constants. The results confirmed that the elaborated nanomaterials present an important potential as sorbents for lead removal from water.

[1] R. Rusmin *et al*, Chemosphere 186, 1006 (2017).
[2] A. Awward, *et al,* Am. J. . Chem. 2, 238 (2012).
[3] M. B. Gawande, *et al,* RSC Advances 2, 6144 (2012).

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ELECTROCHEMICAL DETECTION OF TRICLOSAN IN TOOTH PASTE AND LAKE WATER SAMPLES BY MEANS OF GOLD NANOPARTICLE-POLYIONIC LIQUID NANOCOMPOSITE ELECTRODE

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Indium-doped tin oxide (ITO) substrates modified with Au nanoparticle-poly(ionic liquid) (Au-PIL) nanocomposite films are employed for the voltammetric detection of triclosan (TCS) in lake water and toothpaste samples. The electroanalytical performance evaluated by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and differential pulse voltammetry (DPV), shows the modified electrode oxidizes TCS at much higher oxidation currents than bare ITO. At optimized conditions, the analytical method is linear ($R^2 > 0.99$) in the selected working range (10 - 60 µmol L^{-1}), presents a sensitivity of 57.1 µA cm^{-2}/mol L^{-1}·and a limit of detection of 0.098 µmol L^{-1} (28.3 µg L^{-1}). TCS determinations are successfully carried out in spiked lake water samples showing that the electrode response is not affected by such a complex matrix. The concentration of TCS found in a commercial brand toothpaste, simultaneously determined by voltammetry and HPLC, is similar (95% confidence level, t-test) between both techniques and comparable to that described in the product package.

[1] Zheng, J., Zhang, M., Ling, Y., Xu, J. & Hu, S. Fabrication of one dimensional CNTs/Fe3O4@PPy/Pd magnetic composites for the accumulation and electrochemical detection of triclosan. *J. Electroanal. Chem.* (2018).

[2] Wu, T., Li, T., Liu, Z., Guo, Y. & Dong, C. Electrochemical sensor for sensitive detection of triclosan based on graphene/palladium nanoparticles hybrids. *Talanta* 164, 556–562 (2017).

[3] Li, B., Qiu, Z., Wan, Q., Liu, Y. & Yang, N. B-Cyclodextrin Functionalized Graphene Nano Platelets for Electrochemical Determination of Triclosan. *Phys. Status Solidi Appl. Mater. Sci.* 211, 2773–2777 (2014).

[4] M.L. Yola, N. Atar, T. Eren, H. K.-M. RSC Advances Sensitive and selective determination of aqueous triclosan based on gold nanoparticles on polyoxometalate / reduced graphene oxide nanohybrid. 65953–65962 (2015).

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Control of Monolayer $MgCl_2$ Electronic Properties Through Substitutional Doping of Nonmetals and Transition Metals

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In the field of nanoelectronics, two-dimensional materials represent today a very promising platform for new devices with applications that until not so far were considered unfeasible. Specifically, the isolation of graphene and MoS_2 sheets, made possible applications in the field of spintronics and valleytronics that once were considered impractical. However, most of these materials in its pristine form impose some limitation to make their applications available. One alternative to overcome such problem is by doping already known monolayers and tailor some of its intrinsic chemical and physical properties. In this work we study the control of the fundamental electronic properties of two-dimensional $MgCl_2$ by doping it with a variety of atoms. We performed density function theory (DFT) calculations on 2D $MgCl_2$ doped with nonmetals (H, B, C, N, O, F) and transition metal atoms (V, Cr, Mn, Fe, Co, Ni) that substituted a Cl atom. Our results show that the stability of functionalized $MgCl_2$ by substitutional doping of nonmetals has a higher stability than that by the adsorption process. In addition, for the substitution with nonmetals, we found that only the C and N dopants break the symmetry between up and down spin states, and change the monolayer from an insulator to a half-metal. The substitution by C, turns it into a semiconductor for spin up and a metal for spin down, while by N, becomes a semiconductor for spin down and metal for spin up states. As for the transition metal dopants, all of them gave some magnetic moment to the monolayer, and turned it into a half-metal. For the V dopant, the $MgCl_2$ became a metal for spin up states and a semiconductor for spin down. For the others, the spin up states represent the electronic configuration of a semiconductor, and for spin down, of a metal.

[1] E. Stavrou, Y. Yao, J. M. Zaug, S. Bastea, B. Kalkan, Z. Konôpková and M. Kunz, Sci. Rep., 6, 30631 (2016)
[2] Partin, D. & O’Keeffe, M. J. Solid State Chem. 95, 176 (1991)

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Graphene/(di-methyl di-dodecyl quartenary ammonium) LBL for non-specific impedimetric sensor.

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The present work shows the initial work on the development of non-specific sensors for electronic olfaction. The present results show the sensibility and stability of the Graphene/di-methyl di-dodecyl bromide (DMDDB) LBL film for ethanol, acetone, THF and water. The exfoliation of graphene was performed using a low potency bench ultrasound 60 W (70 h.) in a dispersion of 1 g of bare graphite in N-methyl pirrolidone (NMP). The film was deposited by dip-coating technic from NMP and spin coated, at 300 rpm, for 30 seconds. Then, the film was left to dry at 25 º C. As a second layer DMDDB was deposited by dip-coating onto the as-deposited graphene and spin-coated for 30 seconds and left to dry at 25 º C, at room conditions. The experimental setup for sensorial assays consists of a flux of air (1scm/min) bubbled in pure above cited solvents and conducted to a sensorial thorough PTFE tube. Once in electrical contact, the film has the changes of the impedance values monitored in real time inside a sensorial glass chamber. The results show a dramatic fall of impedance upon exposition to the vapor of above cited solvents in air flux. Bare graphene films, in turn, shows a moderated rising of the impedance. It suggests the successful of LBL procedure for modification and improvement of the sensibility and stability of the bare graphene film. Despite the non-specific character of the sensor, different responses were verified for each solvent, showing a great potential for application in olfactive devices. www.3nano2019.com for the program and dates). Please send it to 3nanoabstracts@gmail.com.

[1] DA SILVA, Mauro J. Calorim., v. 107, n. 1, p. 257-263, 2012.
[2] CAVALLARI, Marco R. et al. IEEE Sens. J,, v. 17, n. 7, p. 1971-1980, 2017.

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USE OF THE IONIC STRENGTH TO IMPROVE THE COLLOIDAL STATE OF AQUEOUS MAGNETIC FLUIDS

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Magnetic nanocolloids are ultra-stable colloidal dispersions of magnetic nanoparticles in a specific carrier liquid [1]. Recently, cobalt ferrites ($CoFe_2O_4$) have been widely studied for their potential application in diverse areas such as biotechnology, biomedicine, for example, for cleaning wastewater through adsorption or as a vector of drugs to treat cancer cells. Thus, this work synthesized a magnetic ferrofluid with nanoparticles based on cobalt ferrite with a maghemite surface layer (γ-Fe_2O_3), by the hydrothermal co-precipitation method [2], in which they were dispersed in an aqueous medium. The nanoparticles then undergo the process of functionalization and separation in size. The magnetic ferrofluid with electric double layer nanoparticles (EDL-MF) was submitted to several characterization techniques. With the data obtained by XDR and MET it was possible to verify the size, structure and shape of the nanoparticles, besides observing that the size separation process was effective. With the AAS we were able to determine the proportion of elements of the core/shell structure and through SAXS, we analyze the balance of forces of the ferrofluid. This study aimed at a dispersion in a Deep Eutectic Solvent (DES), considered a green solvent because it is biodegradable, non-toxic, besides having a high thermal stability, among other characteristics that can make viable applications in vivo for being biocompatible [3].

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References:

[1] Berkovski, B. M. Magnetic fluids and applications handbook; Unesco series of learning materials; New York : Begell House, 1996, 2001.
[2] Tourinho, F. A.; Franck, R.; Massart, R. ;Journal of Materials Science 1990, 25, 3249.
[3] Zhang, Q.; De Oliveira Vigier, K.; Royer, S.; Jérôme, F. ;Chemical Society Reviews 2012, 41, 7108.

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PHOTOCHEMICAL SYNTHESIS OF SILVER NANOPARTICLES STABILIZED BY GRAPHENE OXIDE-POLY(ETHYLENE IMINE) NANOCOMPOSITE

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Nanocomposites based on silver nanoparticles (AgNP) and graphene oxide (GO) are promising materials for many applications, especially in enhancement of Raman scattering (SERS) and phototherapy platforms for câncer treatment. Convencional chemical synthesis of metallic nanoparticles invariably use environmentally hazardous reducing agentes. This study describes an alternative benign and environmentally friendly method in which the chemical reducing agent is replaced by UV 254 nm/16 W irradiation. An aqueous colloidal suspension of carboxylated GO covalently functionalized with branched poly(ethylene imine) (PEI) is mixed with $AgNO_3$ and further irradiated by UV radiation for a period of 30 minutes. The produced Ag-GO-PEI nanocomposites suspensions, exhibit a typical plasmonic band located at 405 nm, confirming the succesful formation of AgNP. Further, the amount of AgNP in the nanocomposites can be precisely tuned by adjusting the $AgNO_3$ to GO-PEI molar ratio, from 5 up to 100. All samples have positive zeta potential and hydrodynamic sizes below 150 nm. Monitoring the formation of AgNP by UV-Vis spectroscopy reveals a first order kinetics process, in which the rate of AgNP formation is increased with the $AgNO_3$ to GO-PEI molar ratio. The photochemical synthesis performed with individual carboxylated GO can not produce AgNP without instantaneous sedimentation. Furthermore, attempts to produce AgNP in dark conditions or in ambiente light are also unsuccessful. These results ratify that previous functionalization of GO with PEI and the use of UV radiation are fundamentally relevant for this method.

[1] Teixeira, P.R.; Santos, M.S.C.; Silva, A. L. G.; Báo, S. N.; Azevedo, R. B.; Sales, M. J. A.; Paterno, L.G. Coll. Surf. B, 148, 317-323 (2016).
[2] Costa, I. A.; Maciel, A. P.; Sales, M. J. A.; Rivera, L. M. R.; Soler, M. A. G.; Pereira-da-Silva, M. A.; Moreira, S. G. C. J. Phys. Chem. C, 122, 24110-24119 (2018).

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Effect of shell thickness on the magnetic properties of $CoFe_2O_4@\gamma\text{-}Fe_2O_3$ core/shell nanoparticles

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Materials at the nanometric scale have shown promising for several applications because of their striking magnetic, physical and chemical properties [1]. Among them we highlight, the magnetic ferrofluids based on ferrites nanoparticles. Magnetic ferrofluids are magnetic nanoparticles dispersed in a carrier liquid, these fluids can be used to deliver packages such anticancer drugs.

Ferrofluids based on core/shell nanoparticles of $CoFe_2O_4@\gamma\text{-}Fe_2O_3$ are prepared by a hydrothermal coprecipitation method [2]. In order to observe the influence of the shell thickness on the magnetic properties we vary the time of superficial treatment from 15 and 120 min.

The structural and morphological properties of these nanoparticles are investigated by X-ray diffraction and Transmission Electronic Microscopy (TEM) experiments. The spinel structure of the NPs is confirmed, and the mean size diameter is determined from X-ray measurements. The size distribution and shape are investigated by TEM images. The mean size diameter of the samples investigated here is ~3 nm. The chemical composition is investigated by atomic spectroscopy absorption (AAS). The chemical tritation results have shown a considerable reduction on the volume fraction of divalent metal X_M after two hours of surface treatment treatment from 0.33 to about ~0.10.

We focus here on the magnetic properties of these samples. First we investigate the low field magnetization dependence with the temperature. We observed a decreasing on the blocking temperature as a function of the shell thickness. In the future it would be interesting to investigate the magnetic shell layer of the samples investigated here using Mossbauer Technique. The EB properties have already been investigated previously as a function of the interaction of the magnetic nanoparticles and core composition [3,4]. Here we will investigate the EB properties as a function of the shell thickness.

[1] T. Pedro; M. Morales; S. Verdaguer; T. Carreño and C. Serna, " The preparation of magnetic particles for applications in biomedicine," J. *Phys. D: Appl. Phys* vol. 36, no. 13, pp. 182-197, 2003.
[2] F. A. Tourinho, R. Franck and R. Massart, " Synthesis and magnetic properties of manganese and cobalt ferrite ferrofluids," *Progr. Colloid. Polym. Sci*., vol. 79, p. 128-134, 1989.
[3] R. Gomes; F. Silva; R. Aquino; P. Boinville; F.A. Tourinho; R. Perzynski; J. Depeyrot, "Exchange bias of $MnFe_2O_4@\gamma Fe_2O_3$ and $CoFe_2O_4@\gamma Fe_2O_3$ core-shell nanoparticles," *J. Mag. Mater.*, vol. 368, p. 409-414, 2014.
[4] F. G. Silva; R. Aquino; F. A. Tourinho; V. I. Stepanov; Y. L. Raikher; R. Perzynski and J. Depeyrot," The role os magnetic interactions in exchange bias properties of $MnFe_2O_4@\gamma\text{-}Fe_2O_3$ core-shell naoparticles," J. *Phys. D: Appl. Phys* vol. 46, no. 28, pp.9 , 2013.

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ANISOTROPY OF THE THERMODIFFUSION UNDER MAGNETIC FIELD IN IONIC LIQUID BASED FERROFLUIDS

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Ferrofluids based on Ionic Liquids (ILs) are new materials, recently developed for thermoelectric low grade energy harvesting [1]. They can be stabilized in a wide range of nanoparticle volume fractions (0.2vol% $\leq \Phi \leq$ 15vol%) and temperatures (295 K $\leq T \leq$ 473K) [2,3]. We investigate here the properties of concentrated dispersions of maghemite nanoparticles (NPs) in two IL model-systems, namely in ethylammonium nitrate (EAN) [4] and 1-Ethyl-3-methylimidazolium bistriflimide (EMI-TFSI) [3]. In the first system, the NPs (≈ 7 nm) are citrate-coated with Na^+ counter-ions, while they are slightly larger (≈ 9 nm) and hydroxyl-coated with $SMIM^{\pm}$-$TFSI^-$ counter-ions in the second system. A Forced Rayleigh scattering experiment under an applied magnetic field [5,6] allow to probe the anisotropy of the NP Soret coefficient and their diffusion coefficient at various Φ and T. The results are analysed according to the model developed in [7].

[1] T.J. Salez et al Nanoscale Advances 1, 2979 (2019)
[2] M. Mamusa et al Faraday Discussions 181, 193 (2015)
[3] J.C. Riedl et al (submitted). On chemrxiv, doi:10.26434/chemrxiv.9817208
[4] K. Battacharya et al (submitted)
[5] M. Kouyaté et al Phys. Chem. Chem. Phys. 21, 1895-1903 (2019)
[6] M. Sarkar et al EPJE 42,72 (2019)
[7] T.J. Salez et al Entropy 20, 405 (2018)

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A monotonic gap tunning through changes in aromaticity for the cove-type graphene nanoribbon

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Graphene is widely known for its promising electronic properties[1]. However, since graphene lacks a bandgap, this material can not be used in semiconductor applications. Gap opening can be achieved by reducing graphene into nanoribbons (GNR). Recently, it was proposed a GNR synthesized through a bottom-up and liquid-based process. This material was described as well defined, unusually long (>200nm) with a cove-type periphery proper for large-scale production. Despite its synthesis advantages, a viable gap tuning procedure is mandatory to successfully introduce GNRs in the industry. In this work, we report an alternative method to smoothly tune the energy band gap by systematically changing the cove-type edge termination. The procedure was applied to several cove-type GNRs with different width sizes. The GNRs were simulated through an extended two-dimensional SSH model[3] with a tight-binding effect (electron-phonon coupling). Static configurations were built using a self consistent field method. It was observed that changing the cove-type periphery led to a loss in aromaticity. This structural change induced a monotonic decay of the gap magnitude. The discovered tuning procedure might assist the design of new technologies based on this promising material. The description contributes as well for the theoretical understanding of confined quantum systems.

[1] M. J. Allen, V. C. Tung, Chem. Rev., 110, 132–145(2010)
[2] A. Narita, X. Feng, Nature Chemistry, 6, 126–132(2014)
[3] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett., 42, 1698-1701(1979)

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MODELING OF THE FIELD-INDUCED RESPONSE OF A MAGNETIC POLYMERSOME

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Submicron capsules with double-layer polymer membranes stuffed with magnetic nanoparticles (MNPs) are known in the literature as *magnetic polymersomes* (MPSs) [1]. Due to the MNPs in their membranes, MPSs could be driven by a field gradient that makes them convenient carriers for drug delivery since the inner cavity is available for any necessary cargo. Our work is concerned with the physics of another method of MPSs usage in cellular medicine. The key point there is the ability of MPSs to deform under a uniform field. The field orients the magnetic moments of MNPs and makes them to unite in chains. Being arc-like due to the confinement, the chains strive to straighten along the field, and by that force the MPS to elongate. Thus, one gets a nanodevice generating localized mechanical forces on the surface of an individual cell. This stimulation opens way to launch mechano-biochemical processes or even to drill a hole in the cell membrane.

In the model, the MPS is presented as two nested "particulate" (in coarse-grained sense) flexible shells between which a monolayer of magnetic nanoparticles is enclosed [2]. The particles interact as soft dipolar spheres. The membrane boundaries are impenetrable for them and are linked in such a way that they keep the intramembrane thickness equal to its equilibrium value. The response of an MPS to a uniform magnetic field is calculated in the framework of coarse-grained molecular dynamics by integrating equations of motion of all the elements of the system. The effect of field-induced MPS elongation was studied at different filler fractions, intensity of MNPs' interaction and strength of coupling between the membrane boundaries.

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[1] S. Lecommandoux, O. Sandre, F. Chécot, J. Rodriguez-Hernandez, R. Perzinski, Advanced Materials 17, 712 (2005)
[2] A. Ryzhkov, Yu. Raikher, Nanomaterials 8, 763 (2018)

LIPOSOMES USE IN DIABETIC WOUNDS TREATMENT: A SYSTEMATIC REVIEW

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Liposomes have been considered excellent nanomaterials for application in wound healing [1]. These materials have been considered ideal drug delivery vesicles due to their biocompatibility, non-immunogenicity and biodegradability. Another advantage of the use of liposomes derives from the possibility of associating hydrophobic and hydrophilic bioactive molecules and this further the penetration of these molecules in the skin. Liposomes can also be used for gradual and sustained release of biomolecules in wounds, thus promoting better wound healing [2], [3]. Thus, the objective of this study was to show, through database searches, the scientific production on the use of liposomes in the treatment of diabetic ulcers. For this, systematic searches were performed in nine databases for publications in the last 10 years. English language keywords were used and searches were performed in the Title, Abstract and Keywords fields, except when this option did not exist. Subsequently, the duplicates were excluded and the title and summary of the resulting publications were read for data extraction. 259 works were obtained and it was observed that from 2015 to 2019 was the period in which there was the largest increase in the number of publications, (73%). Review articles led the ranking of publication types (49.8%), followed by research articles (35.5%). Only 15 research articles were included for analysis, with the United States and India being the most published countries (four papers each). Of the articles included, almost 70% were related to in vivo trials. Most authors used liposomes in solution form corresponding to 10 publications; 9 did not specify the type of liposome used and 12 performed topical application of the treatment. Only one article was a clinical trial, a case report. It is concluded that research relating liposomes to promote diabetic wound healing has grown substantially, although there are still few studies in the area, especially clinical trials. The most commonly used forms of treatment are topical application to wounds and liposomes in solution.

[1] S. Hamdan *et al.*, “Nanotechnology-Driven Therapeutic Interventions in Wound Healing: Potential Uses and Applications,” *ACS Cent. Sci.*, vol. 3, no. 3, pp. 163–175, Mar. 2017.
[2] M. Nounou, L. El-Khordagui, N. Khalafallah, and S. Khalil, “Liposomal Formulation for Dermal and Transdermal Drug Delivery: Past, Present and Future,” *Recent Pat. Drug Deliv. Formul.*, vol. 2, no. 1, pp. 9–18, May 2008.
[3] J. Rodrigues da Silva and F. de Matos da Silva, “Nanosistemas lipídicos e poliméricos para aplicação tópica no tratamento de feridas,” vol. 25, pp. 7–25, 2018.

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