VII Iberian Meeting on Colloids and Interfaces (RICI7)

Madrid, July4th – July7th, 2017

Facultad de Ciencias Químicas

Universidad Complutense de Madrid

RICI 7

ABSTRAC BOOK

Scientific Committee

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Scientific Program

Tuesday, 4th July 2017

15:00-17:30 Registration

17:30-19:00 Welcome Party

Wednesday, 5th July 2017

8:00-8:40 Registration

8:40-9:00 Opening *(Aula Magna)*

9:00-9:45 **PL-1** *(Aula Magna)*
Photoacoustic effect: A new way of interacting with the micro- and nano-world.
F. Galisteo-González
Chairman: Francesc Mas

9:50-13:30 Parallel Sessions

Room 1 (QC23)

Chairman: Andrés Guerrero Martínez

9:50-10:20 **IL-1** **Plasmonics for biological applications based in interfacial self-assembly**
Juan J. Giner-Casares

10:20-10:40 **O-1** **Copper sulfide nanocrystals@graphene: synthesis and photocatalytic activity**
Ana C. Estrada, Joana Lopes, Tito Trindade

10:40-11:00 **O-2** **Synthesis, characterization and evaluation of magnetic doped ferrites as potential therapeutic tools**
Alberto Pardo, Mateo Blanco-Loimil, Beatriz Pelaz, Pablo del Pino, Francisco Rivadulla, Wolfgang Parak, Silvia Barbosa, Pablo Taboada

11:00-11.30 *(Building C) Coffee Break*

Chairman: Conxita Solans

11:30-11:50 **O-3** **Raman imaging for the investigation of antimicrobial fabric dyeing**
Sara Fateixa, Manon Wilhelm, Helena I. S. Nogueira, Tito Trindade

11:50-12:10 **O-4** **Versatile magnetic biohybrid nanosorbents for the removal of herbicides from water**
Tiago Fernandes, Sofia F. Soares, Tito Trindade, Ana L. Daniel-da-Silva

12:10-12:30 **O-5** **Gold-based hybrid nanoplatforms as tools for oncogenic pathway inhibition of aggressive tumors through a combinatorial multi-therapeutic approach.**
E.Villar-Álvarez, Irene Golán-Cancela, Baltazar Hiram-Leal, Raquel Martínez-González, Silvia Barbosa, J. ACostoya, Pablo Taboada

12:30-12:50 **O-6** **A problem with solution: Development of lipid-based colloidal nanocarriers for encapsulation of compounds with weak bioavailability**
T. Soares, M. Lúcio, A. C. P Dias, M. E. C. D. Real Oliveira

12:50-13:10 **O-7** **Hybrid nanoparticles for oral drug administration**
Raquel da Ana, Ana Fortuna, Maria Mendes, Amílcar Falcão, João Sousa, Alberto Pais, Carla Vitorino

13:10-13:30 **O-8** **Development of lipid-based colloidal nanocarriers for topical application of acyclovir**
Juliana Silva, C. Martins Lopes, J.A.M. Catita, M.E.C.D. Real Oliveira, Marlene Lúcio

Room 2 (QC25)

Chairman: Juan José Giner Casares

9:50-10:20 **IL-2** **Synthesis and Optical Studies of Silica Encapsulated Quantum Dots During Optical Trapping**
Beatriz H. Juárez

10:20-10:40 **O-14** **Ionic Surfactant-Carbon Nanotube Interactions. Use of Ion-Selective Electrodes**
M. López-López, E. Bernal, M.L. Moyá, J.A. Lebrón, P. López-Cornejo

10:40-11:00 **O-15** **Cationic colloidal system based on amino acid-based surfactants: characterization, antimicrobial properties and cytotoxicity**
L. Pérez, R. Pons, A. Pinazo, M.A. Manresa, C. Moran

11:00-11.30 *(Building C) Coffee Break*

Chairman: Emilio Aicart

11:30-11:50 **O-16** **Modulating supramolecular nanostructures: a free energy oriented approach**
Tânia. F .G. G. Cova, Sandra. C. C. Nunes, Alberto. A. C. C Pais

11:50-12:10 **O-17** **Stoppering/unstoppering of a rotaxane formed between an N-heterocycle ligand containing surfactant:β-cyclodextrin pseudorotaxane and pentacyanoferrate(II) ions**
V. I. Martín, P. López-Cornejo, M. López-López, M. L. Moyá, F.J. Ostos

12:10-12:30 **O-18** **Aggregation of cyclodextrins: insights into dynamic properties from NMR**
A.J.M. Valente, D. Murtinho, R.A. Carvalho, O. Söderman

12:30-12:50 **O-19** **Molecular self-assembly of thiacyanine dyes into liquid crystals and silicatropic materials**
José Rodrigo Magaña, Gordon J.T. Tiddy, Carlos Rodríguez-Abreu

12:50-13:10 **O-20** **Tubular Nanostructures and Protein Binding in Lysine-based Surfactants**
Isabel S. Oliveira, Mikail Lo, M. João Araújo, Eduardo F. Marques

13:10-13:30 **O-21** **Self-Assembly of Gold Nanoparticles based on Supramolecular Concepts**
Andrés Guerrero Martínez

13:30 End Parallel Sessions

13:30-15:00 *Lunch*

15:00-15:45 **PL-2** *(Aula Magna)*
Colloid Particles at a Range of Fluid-Fluid Interfaces
Bernard P. Binks
Chairman: Francisco Ortega

15:45-17:10 *(Building C) Poster Session+Coffee Break*

17:15-19:00 Parallel Sessions

Room 1 (QC23)

Chairman: Bruno Silva

17:10-17:40 **IL-3** **Role of counter-ion and helper lipid content in the design and properties of nanocarrier systems: a biophysical study**
M. Elisabete C.D. Real Oliveira

17:40-18:00 **O-9** **Miniemulsion polymerization as a synthetic platform for structure control of multifunctional polymer/metaloxide hybrid nanoparticles**
Olaia Álvarez-Bermúdez, Katharina Landfester, Rafael Muñoz-Espí

18:00-18:20 **O-10** **Highly Controlled Synthesis of Gold Nanostars in Microdroplets**
S. Abalde-Cela, P. Taladriz-Blanco, C. Abell

18:20-18:40 **O-11** **Crystal Engineering of Nano-Micro Particles in Polar Media**
Ana Querejeta-Fernández, Beatriz Rivas-Murias, Miguel Correa-Duarte, Verónica Salgueiriño

18:40-19:00 **O-12** **Drug biophysical profiling using lipid-based colloidal nanosystems and human serum albumin as biomimetic interfaces**
E. Fernandes, M. E. C. D. Real Oliveira, S. Benfeito, F. Cagide, F. Borges, M. Lúcio

Room 2 (QC25)

Chairman: Pablo Taboada

17:10-17:40 **IL-4** **IESMAT: Scientific instrumentation for characterizacion of COLLOIDS**
Jesús Puebla

17:40-18:00 **O-22** **Large-Scale Plasmonic Pyramidal Supercrystals via Templated Self-Assembly of Monodisperse Gold Nanospheres**
Guillermo González-Rubio, Christoph Hanske, Cyrille Hamon, Pilar Formentín, Evgeny Modin, Andrey Chuvilin, Andrés Guerrero-Martínez, Lluis F. Marsal, Luis M. Liz-Marzán

18:00-18:20 **O-23** **Magnetic Microdockers**
F. Martínez-Pedrero, H. Massana, E. Navarro-Arguemí, A. Ceber, I. Pagonabarraga, P. Tierno

18:20-18:40 **O-24** **Self-Assembly of Poly(N-Isopropylacrylamide-Methacrylic Acid) Microgels In Water**
Gema Marcelo, Laurinda R. P. Areias, Ermelinda Macoas, Francisco Mendicuti, Mercedes Valiente, J. M. G. Martinho, José Paulo S. Farinha

18:40-19:00 **O-25** **Surface coverage and competitive binding of polymer and protein on carbon nanotubes**
Ricardo Fernandes, Oren Regev, Istvan Furó, Eduardo F. Marques

19:00 End of Parallel Sessions

Thursday, 6th July 2017

9:00-9:45 **PL-3** *(Aula Magna)*
Proteins on membrane interfaces: Structure and dynamics of lipid-protein fibers from advanced FRET methodologies and microscopy
Manuel Prieto
Chairman: Francisco Monroy

9:50-13:30 Parallel Sessions

Room 1 (QC23)

Chairman: Ramón González Rubio

9:50-10:20 **IL-5** **From macroscopic molecular gels to molecular nanoparticles for transport and delivery of actives**
Juan F. Miravet

10:20-10:40 **O-26** **Surface Dilational Elasticity of Monolayers Adsorbed from Polyelectrolyte and Surfactant Mixtures**
Andrew Akanno, Eduardo Guzmán, Francisco Ortega, Ramón G. Rubio

10:40-11:00 **O-27** **Combining miniemulsion and solvothermal conditions for the synthesis of complex inorganic systems**
Rafael Muñoz-Espí, Alice Antonello, Katharina Landfester, Silvia Gross

11:00-11.30 *(Building C) Coffee Break*

Chairman: Tito Trindade

11:30-11:50 **O-28** **Molecular Trends in Surfactant-Assisted Dispersions of Carbon Nanotubes**
Bárbara Abreu, Ricardo M.F. Fernandes, Matat Buzaglo, Oren Regev, István Furó, Eduardo F. Marques

11:50-12:10 **O-29** **Modelisation of the evaporation of a complex sessile droplet**
L. Perrin, S. Semenov, R.G. Rubio, M. Velarde

12:10-12:30 **O-30** **Dissolution state of cellulose in aqueous systems**
Luis Alves, Bruno Medronho, Filipe E. Antunes, Daniel Topgaard, Björn Lindman

12:30-12:50 **O-31** **Study of the adsorption of polyelectrolyte-surfactant mixtures at the water/vapor interface by neutron reflectivity and surface tension measurements**
Laura Fernández-Peña, Andrew Akanno, Eduardo Guzmán, Sara Llamas, Aurelio G. Csaky, Richard A. Campbell, Reinhard Miller, Francisco Ortega, Ramón G. Rubio

Chairman: Francisco Galisteo González

12:50-13:10 **O-32** **Phase transitions in fatty acids/alcohols Langmuir monolayers: Interfacial shear rheology results**
Javier Tajuelo, Francisco Ortega, Ramón G. Rubio, Eduardo Guzmán, Miguel A. Rubio

13:10-13:30 **O-33** **Gemini Cationic Surfactants: Studying its Adsorption at Air/Water Interface and its micellization by ITC Calorimetry**
V. Domínguez, J. Sabín, G. Prieto

13:30-13:50 **O-34** **Emulsions containing essential oils: eco-friendly aqueous formulations of potential biopesticides for insect pest control**
Eduardo Guzmán, Alejandro Lucia, Elisabet L. Afonso, Natalia Sánchez-Arribas, Marina Fernández-Medina, Erica Cordero, Pablo G. Argudo, Francisco Ortega, Ramón G. Rubio

Room 2 (QC25)

Chairman: Manuel Prieto

9:50-10:20 **IL-6** **Lipid nanosystems for therapeutic purposes – biophysical studies as useful tools to understand interactions at the nano–bio interface**
Marlene Lúcio

10:20-10:40 **O-13** **Self-assembledmolecular nanoparticles as new delivery Systems**
Ana Torres-Martínez, Francisco Galindo, Juan F. Miravet

10:40-11:00 **O-36** **Bioreactors Engineered through Microfluidics**
Berta Tinao, Lara H. Moleiro, Sergio A. Ortega, Laura R. Arriaga, Margarita Salas, Francisco Monroy

11:00-11.30 *(Building C) Coffee Break*

Chairwoman: Elena Junquera

11:30-11:50 **O-37** **Layer-by-Layer Polyelectrolyte Microcapsules**
Ana Mateos-Maroto, Sergio Montero López, Marta Ruano Aldea, Eduardo Guzmán, Francisco Ortega, Ramón G. Rubio

11:50-12:10 **O-38** **Hyaluronic Acid-Coated Liquid Lipid Nanocapsules as Delivery Systems Against Pancreatic Cancer Stem Cells**
A. Aguilera-Garrido, F. Galisteo-González, J.A. Molina-Bolívar, J. A. Marchal, T. del Castillo Santaella, J. Maldonado-Vaderrama, M. J. Gálvez-Ruiz

12:10-12:30 **O-39** **May a Policationic Macrocycle Act as a Cationic Bridge Among an Anionic Lipid and a Plasmid DNA to Transfect Cells Efficiently?**
María Martínez-Negro, Ana Barrán-Berdón, Òscar Domènech, Luis García-Río, Conchita Tros de Ilarduya, Emilio Aicart, Elena Junquera

12:30-12:50 **O-40** **Colloidal characterization and in vitro study of olive oil immune-nanocapsules for directed drug delivery**
S. Navarro-Marchal, J.A. Marchal, A.B. Jódar-Reyes, J.M. Peula-García

Chairman: Francisco Monroy

12:50-13:10 **O-41** **Unravelling clathrin-mediated endocytosis**
Armando Maestro, Nathan Zaccai, David Owen, Pietro Cicuta

13:10-13:30 **O-42** **Effect of Cardiolipin on liposomes**
Samuel Salinas-Almaguer, Carlos Ruiz, Francisco Monroy

13:30-13:50 **O-43** **Polymeric particles and membranes for cell encapsulation, proliferation and release**
Eustolia Velázquez, Baltazar H- Leal, Silvia Barbosa, Manuel Altorre-Meda, Pablo Taboada

13:50 End of Parallel Sessions

13:50-15.10 *Lunch*

15:10-15:55 **PL-4** *(Aula Magna)*
Studying the Heat Effect of Nanoparticles for Therapy and Diagnosis
Jesús Martínez de la Fuente
Chairman: Francisco Galisteo González

16:00-16:40 Parallel Sessions

Room 1 (QC23)

Chairwoman: Mercedes Velázquez

16:00-16:20 **O-35** **Phospholipid/Nucleolipid Mixed Films for Guanine Recognition at the Air-Water Interface**
Pablo Gómez-Argudo, Juan J. Giner-Casares, Luis Camacho, M. Teresa Martín-Romero

16:20-16:40 **O-46** **Computer simulations of interaction forces between nanogels**
Manuel Quesada-Pérez, Silvia Ahualli, José Alberto Maroto-Centeno,Alberto Martín-Molina

Room 2 (QC25)

Chairman: Francesc Mas

16:00-16:20 **O-44** **Effect of NaCl on the aggregation behavior of rhamnolipids and implications in their biological activity**
Ana I. Rodrigues, Eduardo J. Gudiña, José A. Teixeira, Lígia R. Rodrigues

16:20-16:40 **O-45** **Gold Nanorods in Surface-Enhanced Raman Spectroscopy as a Toxicological Tool for Cocaine Detection**
Valentina D'Elia, Jorge Rubio Retama, Carmen García Ruiz, Gemma Montalvo

16:40 End of Parallel Sessions

16:40-18:00 *(Building C) Poster Session+Coffee Break*

17:00-19:00 *(Room QC23) Meeting of the GECI*

20:30-… *Social Dinner*

Friday, 7th July 2017

9:00-9:45 **PL-5** *(Aula Magna)*
Multifunctional materials and nanostructures using anodic templates
Joao Pedro Araujo
Chairman: Bruno Silva

9:50-11:00 Parallel Sessions

Room 1 (QC23)

Chairman: Jesús M. de la Fuente

9:50-10:20 **IL-7** **Surface modification with functional alkoxysilanes: a valuable route for selective and effective magnetic nanosorbents**
Ana L. Daniel-da-Silva

10:20-10:40 **O-47** **Microgels obtained in water-in-water (w/w) emulsions**
Y. Beldengrün, J. Aragón, L. Corvo, C. Miquel, M. Ros, J. Esquena

10:40-11:00 **O-48** **Role of charge distribution in the absorption of biomolecules in ionic microgels**
Irene Adroher-Benítez, Arturo Moncho-Jordá, Joachim Dzubiella,

Room 2 (QC25)

Chairman: Alberto Canelas Pais

9:50-10:20 **IL-8** **Multilayered and 3D structures of Bacterial cellulose composites with nanoparticles**
Anna Laromaine

10:20-10:40 **O-49** **Soft self-assembled nanoparticles for gene and drug delivery**
Bruno F. B. Silva

10:40-11:00 **O-50** **PNIPAM-Based Microgels with a UCST Response**
Gema Marcelo, Laurinda R. P. Areias, Maria Teresa Viciosa, J. M. G. Martinho, José

11:00 End of Parallel Sessions

11:00-11.30 *(Building C) Coffee Break*

11:30-13:15 *(Aula Magna)*
Symposium in memoria of Elvira Rodenas
Chairman: Francisco Ortega

13:15-14:00 **PL6** *(Aula Magna)*
Closure Lecture: Surfactant self-assemblies: Key role in low-energy emulsification
Conxita Solans
Chairwoman: Jacqueline Forcada

14:00-… *(Aula Magna) Conclusions*

Poster Session (Wednesday, 5th July 2017, 15:45-17:10 and Thurday, 6th July 2017,16:40-18:00)

P-1 Release of acyclovir from polymeric nanofibers: comparing aqueous versus membrane-water interfaces kinetics
Tiago Costa, Andreia Almeid, José das Neves, Bruno Sarmento, Marlene Lúcio, Teresa Viseu

P-2 Smart drug delivery systems for cancer therapy
Eduarda Bárbara, Rasa Ozolina, Ana M. Carvalho, Telma Soares, Hugo Gonçalves, Jana B. Nieder, M.E.C.D. Real Oliveira, Marlene Lúcio

P-3 Pyrene as fluorescent probe of graphene in aqueous and micellar SDS dispersions
S. Vera, P. Martínez, A.M. Díez-Pascual, M.P. San Andrés, M. Valiente

P-4 Importance of the hydrophobic interactions in the DNA compaction ability of surfactants
M. López-López, M. L. Moyá, F. Sánchez, E. Bernal, A. Sánchez, M. J. Marchena, A. Clavero, P. López-Cornejo

P-5 The concerted action involving conformation and desolvation that makes water-soluble bambusurils unique anion cages
Tânia F .G. G. Cova, Sandra. C.C. Nunes, Alberto. A.C. Pais

P-6 Cellulose as a dispersion stabilizer
Carolina Costa, Björn Lindman, Isabel Mira, Jan-Benjamin Williams, Håkan Edlund, Magnus Norgren

P-7 Hydrophobically-modified chitosan nanovectors for efficient siRNA delivery
Baltazar H. Leal, Josué Juárez, Miguel A. Váldez, Eva Villar-Alvarez, Silvia Barbosa, Pablo Taboada

P-8 Synthesis and characterization of protein-loaded nanocapsules
María Navarro-Poupard, Mozhgan Barami, Beatriz Pelaz, Pablo del Pino, Pablo Taboada

P-9 Evaluation of activity and degradation in biological media of upconverting-based nanoplatforms for theranostic applications
R. Martínez-González, E. Villar-Álvarez, B. Hiram-Leal, M. F. Poupard, B. Pelaz, S. Barbosa, P. del Pino, P. Taboada

P-10 Two-dimensional self-assembled arrays of metallic nanoparticles for biotechnological applications
Mateo Blanco Loimil, Alberto Pardo, Silvia Barbosa,Pablo Taboada, Víctor Mosquera

P-11 Studies on the interaction of cationic polymers with microorganisms: development of photobactericidal surfaces
C. Arnau del Valle, C. Felip-León, V. Pérez-Laguna, M. I. Millán-Lou, J. F. Miravet, M. Mikhailov, M. N. Sokolov, A. Rezusta-López, F. Galindo

P-12 Deamidation of pseudopeptidic supramolecular gels and its application to controlled release
César A. Angulo-Pachón, Diego Navarro-Barreda, Celia M. Rueda, Francisco Galindo and Juan F. Miravet

P-13 Surface properties of conducting polymer films
Ángel Arias, David López, M.D. Merchán, M.M. Velázquez

P-14 Surface properties of Nanocomposites for capturing of CO_2
Sara Rodríguez García, David López-Díaz, M.D. Merchán, M.J. Sánchez Montero, M.M. Velázquez

P-15 Control over phase synchronisation in rotor models of motile cilia
Armando Maestro, Nicolas Bruot, Jurij Kotar, Nariya Uchida, Ramin Golestanian, Pietro Cicuta

P-16 PLGA nanoparticles for delivery of Bone Morphogenetic Protein and biofunctionalization of Titanium surfaces
Teresa del Castillo, Ana Belén Jódar-Reyes, Inmaculada Ortega-Oller, Miguel Padial, Pablo Galindo, José Manuel Peula-García

P-17 Optimized surfactant/polymer interactions for the improvement of detergent efficiency
Solange S. Magalhães, Luís Alves, Marco Sebastião, Bruno Medronho, Filipe E. Antunes

P-18 Study of phase separation in a negatively charged colloid / polymer system
Mikheil Kharbedia, Eduardo Enciso, Francisco Monroy

P-19 Hyaluronic Acid-Human Serum Albumin (HAS) Complexes at Fluid Interfaces
Olalla Olea Romacho, Julia Maldonado-Valderrama, Miguel Ángel Cabrerizo-Vílchez, María José Gálvez-Ruiz

P-20 Surfactant-assisted exfoliation of graphite into graphene: dispersibility studies and structural characterization
Bárbara Abreu¸ Jorge Montero, Matat Buzaglo, Oren Regev, Eduardo F. Marques

P-21 Bioreducible polycation-DNA complexes
Filipe Coelho, Eduardo F. Marques, Bruno F. B. Silva

P-22 Raman studies on graphene-based materials doped with metal sulfides
Joana L. Lopes, Ana C. Estrada, Tito Trindade

P-23 Towards a realistic modelling of protein diffusion in polymer crowded media
Pablo M. Blanco, Sergio Madurga, Josep Lluís Garcés, Francesc Mas

P-24 Cationic lipid nanoparticles for topical drug administration
Daniel Magano, Bárbara Ramalho, Cátia Ribeiro, Joana Nova, Alberto Pais, Carla Vitorino

P-25 Serine based gemini lipid nanoparticles for glioblastoma treatment
Maria Mendes, Lídia Gonçalves, Ana Miranda, António Almeida, João Sousa, Eduardo Marques, Alberto Pais, Carla Vitorino

P-26 Molecular dynamics simulations on glioblastoma: Blood brain barrier mimicry and interactions with chemotherapeutic drugs
Ana Miranda, Tânia Cova, Maria Mendes, João Sousa, Carla Vitorino, Alberto Pais

P-27 Magnetic quaternized chitosan hybrid nanoparticles: potential prospects for the uptake of pharmaceuticals from water
Sofia F. Soares, Tiago Fernandes, Margarida Sacramento, Tito Trindade, Ana Daniel-da-Silva

P-28 Previous Steps to *invivo* Studies: Physicochemical and Biological Characterization of a Cationic Gemini Lipid/DOPE-plasmid DNA Lipoplex
NataliaSánchez-Arribas, MaríaMartínez-Negro, Conchita Tros de Ilarduya, EmilioAicart, Elena Junquera

P-29 Spectroscopic characterization of biomimetic light harvesting complexes
Sergio A. Ortega, LauraR.Arriaga, FranciscoMonroy

P-30 Catanionic Vesicles Composed of Threonine-based Surfactants: PhaseBehavior and Microstructure
Isabel S. Oliveira, CristianaSantos, M.Luísa do Vale, Eduardo F. Marques

P-31 Magnetite-supported gold nanostarsforSERSdetectionof antibiotics
Paula C. Pinheiro, SaraFateixa, Tito Trindade

P-32 Photothermal conversion efficiency and cytotoxic effect of gold nanorods stabilized with chitosan, and overcoated with alginate or PVA
M. Almada, B.H. Leal-Martínez, P. Taboada, N. Hassan, A. Topete, M.G. Burboa Zazueta, M.A.Valdez, J. Juárez

PLENARY LECTURES

Photoacoustic effect: A new way of interacting with the micro- and nano-world.

F. Galisteo-González[1,2] and F. M. Goñi[1]
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The photoacoustic effect consists of the formation of sound waves following light absorption by a material upon exposure to short and intense light pulses. This phenomenon was first described by Alexander Graham Bell in 1880 and studied by eminent scientists like Lord Rayleigh, Tyndall and Röntgen, among many others. Soon it became clear that the main possibilities of this technique laid upon spectroscopy: the absorption of light and subsequent emission of sound waves depended on the illuminated material nature. In the seventies, with the arrival of technological improvements in light sources and sound transducers, the technique was extended to materials imaging and, later on, to biological imaging. It is now considered one of the more exciting biomedical imaging techniques of the decade [1].

All of these applications of the photoacoustic effect, nevertheless, lay on the same principle: to register the produced sound waves and extract information from them. A different approximation to this phenomenon, however, was introduced in 1995 by Chen and Diebold [2], when they described that carbon nanoparticles could generate acoustic signals 2.000 times larger than those from dye molecules.

With this highly-absorbing material, the pressure wave can be strong enough to cause mechanical distress in soft matter e.g. cell membranes. At low energy, these mechanical shocks cause disruption of cell membrane integrity, opening transient pores through which compounds of interest may be internalized before the gaps in the membrane are self-repaired. On the other hand, with higher energies, the number and/or extension of the pores may probe to be excessive for the cell to survive, initiating an irreversible process of death. This technique opens an interesting field of mechanical interaction with micro- and nano-systems, and its possible technological applications.

Acknowledgements
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References
[1] S. Manohar and D. Razansky, *Advances in Optics and Photonics*, 8(4) (2016) 586-617
[2] H. X. Chen and G. Diebold, *Science*, 270 (1995) 963–9

Colloid Particles at a Range of Fluid-Fluid Interfaces

Bernard P. Binks
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Many types of colloid particle adsorb at a fluid interface enabling the stabilization of dispersed systems like foams and emulsions. The interfaces include oil-water, air-water, oil-air, oil-oil and water-water.[1] This talk will describe the fundamental properties of some of these interfaces and include the behavior of so-called Pickering emulsions, aqueous and non-aqueous foams, emulsions of two immiscible oils and all aqueous emulsions stabilised by different colloid particles. The preparation of novel materials like dry water, powdered oil and powdered emulsions will be highlighted.

Acknowledgements
This work was supported by the EPSRC, BBSRC, EU and a number of companies.

References
[1]B.P. Binks, Feature Article in *Langmuir*, 2017, in press.

Proteins on membrane interfaces: Structure and dynamics of lipid-protein fibers from advanced FRET methodologies and microscopy

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The aggregation of proteins/peptides on the surface of biological membranes has been receiving growing attention since several studies have reported that lipid/water interfaces can promote the self-assembly of amyloidogenic proteins/peptides into a rich β-sheet structure by acting as two-dimensional conformational catalysts. In addition, it has been proposed that membranes containing negatively charged phospholipids can also trigger rapid "amyloid-like" fiber formation by a variety of non-amyloidogenic proteins/peptides, such as cytochrome *c* and lysozyme. To obtain information about the factors that govern the formation of these supramolecular assemblies, we have been using hen egg white lysozyme as a model protein in our on-going research on lipid-protein interaction studies. Here, we will discuss the molecular details gained about these mesoscopic structures from using a combined set of different fluorescence techniques performed both at the macroscopic and microscopic levels (ensemble-average liposome and single-fiber studies, respectively).Lz interaction with anionic lipid vesicles was first studied using both steady-state and time-resolved fluorescence techniques. The biphasic variation of the mean fluorescence lifetime of Lz fluorescently-labeled with Alexa 488 (Lz-A488) as a function of the surface coverage of the liposomes was quantitatively described by a three-state model. This cooperative model assumes that monomeric Lz molecules partition into the bilayer surface and reversibly assemble into oligomers with k subunits ($k \geq 6$). The global fit was done using the partition coefficients previously determined by FCS and by taking into account electrostatic effects by means of the Gouy-Chapman theory. The oligomer stoichiometry was further narrowed down to $k = 6 \pm 1$ by homo-FRET measurements, which takes into account the binomial distribution of fluorescently-labeled monomers among the oligomers. FLIM-FRET studies and 2PE generalized polarization measurements of Laurdan incorporated in the mixed lipid-protein fibers produced at a low L/P ratio will also be discussed.

Acknowledgements
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Studying the Heat Effect of Nanoparticles for Therapy and Diagnosis

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In the last decades, inorganic nanoparticles have been steadily gaining more attention from scientists from a wide variety of fields such as material science, engineering, physics or chemistry.The very different properties compared to that of the respective bulk, and thus intriguing characteristics of materials in the nanometre scale, have driven nanoscience to be the centre of many basic and applied research topics. Moreover, a wide variety of recently developed methodologies for their surface functionalization provide these materials with very specific properties such as drug delivery and circulating cancer biomarkers detection. In this talk we describe the synthesis and functionalization of magnetic and gold nanoparticles as therapeutic and diagnosis tools against cancer:

-Pseudo-spherical gold nanoparticles derivatized with with fluorescent dyes, cell penetrating peptides and small interfering RNA (siRNA) complementary to the proto-oncogene myc have been tested using a hierarchical approach including three biological systems of increasing complexity: *in vitro* cultured human cells, *in vivo* invertebrate (freshwater polyp, *Hydra*) and *in vivo* vertebrate (mouse) model. Selection of the most active functionalities was assisted step by step through functional testing adopting this hierarchical strategy.[1] Merging these chemical and biological approaches lead to a siRNA/RGD gold nanoparticle capable of targeting tumor cells in lung cancer xenograft mouse model, resulting in successful and significant c-myc oncogene downregulation followed by tumor growth inhibition and prolonged survival of the animals.[2]

-Gold nanoprisms (NPRs) have been functionalized with PEG, glucose, cell penetrating peptides, antibodies and/or fluorescent dyes, aiming to enhance NPRs stability, cellular uptake and imaging capabilities, respectively.[3] Cellular uptake and impact was assayed by a multiparametric investigation on the impact of surface modified NPRs on mice and human primary and transform cell lines.[4,5,6] Under NIR illumination, these nanoprobes can cause apoptosis. Moreover, these nanoparticles have also been used for optoacoustic imaging,[7] as well as for tumoral marker detection using a novel type of thermal ELISA nanobiosensor using a thermosensitive support.[8,9]

-Magnetic nanoparticles functionalized with DNA molecules and further hybridizing with different length fluorophore-modified DNA have allowed the accurate determination of temperature spatial mapping induced by the application of an alternating magnetic field.[10] Due to the design of these DNAs, different denaturalization temperatures (melting temperature, Tm) could be achieved. The quantification of the denaturalized DNA, and by interpolation onto a Boltzmann fitting model, it has been possible to calculate the local temperature increments at different distances, corresponding to the length of each modified DNA, from the surface of the nanoparticles. The local increments achieved were up to 15ºC, and the rigidity conferred by the double strand DNA allowed to evaluate the temperature at distances up to 5.6 nm from the nanoparticle surface.

References

[1] J. Conde, A. Ambrosone, V. Sanz, Y. Hernandez, F. Tian, P. V. Baptista, M. R. Ibarra, C. Tortiglione, J. M. de la Fuente. *ACS Nano*, 2012, 6, 8316.
[2] J. Conde, F. Tian, Y. Hernández, C. Bao, D. Cui, M. R. Ibarra, P. V. Baptista, J. M. de la Fuente. *Biomaterials*. 2013, 34, 7744.
[3] B. Pelaz, V. Grazú, A. Ibarra, C. Magén, P. del Pino, J. M. de la Fuente. *Langmuir*, 2012, 28, 8965.
[4] M.P. Hernández, P. del Pino, S.G. Mitchell, M. Moros, G. Stepien, W. Parak, E. Gálvez, J. Pardo, J.M. de la Fuente. *ACS Nano, 2015*, 9, 52
[5] C. Bao, J. Conde, F. Pan, C. Li, C. Zhang, F. Tian, S. Liang, J.M. de la Fuente, D. Cui. *Nano Research*, 2016, 9, 1043
[6] J. Han, J. Zhang, M. Yang, D. Cui, J.M. de la Fuente. *Nanoscale, 2016*, 492
[7] C. Bao, N. Beziere, P. del Pino, B. Pelaz, G. Estrada, F. Tian, V. Ntziachristos, J. M. de la Fuente, D. Cui. *Small*, 2013, 9, 68.
[8] E. Polo, P. del Pino, B. Pelaz, V. Grazu, J.M. de la Fuente. *Chemical Communications*, 2013, 49, 3676.
[9] G. Alfranca, A. Blein-Rodriguez, S.G. Mirchell, D. Cui, J.M. de la Fuente, submitted
[10] JT Dias, M Moros, P del Pino, S Rivera, V Grazu, JM de la Fuente. Angew Chem Int Ed Engl, 2013, 52, 1152

Multifunctional materials and nanostructures using anodic templates

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The great advances in nanoscience and nanotechnology in the last decade have led to the development of new platforms where all physical properties like size, porosity, geometry and surface functionalization can be controlled at the nanoscale. Self-organized Nanostructuring using template synthesis is a very promising and rapidly expanding field for the preparation of templates and many different ordered nanostructures ranging from the micrometer to few nanometer range [1]. Porous Anodic Aluminum, Titanium, Iron or Hafnium templates with self-organized structures are suitable not only as a well-controlled nanostructured materials for direct applications but also as a templates for preparing two- or three-dimensional arrays of periodic nanostructures.

In this talk, I will focus on the main recent achievements of our research, focused on the implementation and improvement of deposition methods for the synthesis/growth of nanowires, nanotubes and their multifunctional applications ranging from energy to biotechnology.

The opportunities they offer for complementary solid state physics studies will also be discussed.

Acknowledgements
This work was supported by project CERN/FIS-NUC/0004/2015

References
[1] C.T. Sousa, D.C. Leitao, M.P. Proenca, J. Ventura, A.M. Pereira, J.P. Araujo, Applied Physics Reviews 1 (3), 031102

Surfactant self-assemblies: Key role in low-energy emulsification

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The condensation or low-energy emulsification methods are focusing increasing attention because they are advantageous (good size control, mild process conditions) compared to the conventional high-energy methods. The source of the required energy for emulsification, in low-energy methods, rises from the intrinsic chemical energy of the system components which is released during the emulsification process. It is now quite well established that the presence of surfactant molecular assemblies with zero average curvature such as lamellar liquid crystals or bicontinuous microemulsions during the emulsification process play a decisive role in the formation of emulsions with minimum droplet size by low-energy methods based on phase inversion [1]. In this presentation the mechanisms by which nanodroplets are generated by phase inversion emulsification methods will be first discussed. It will follow a description on the use of emulsions obtained by low-energy methods as efficient templates for the preparation of nanostructured materials with controlled and multifunctional properties.

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References
[1] C. Solans, I. Solé, Current Opinion in Colloid & Interface Science 17 (2012) 246–254

INVITED LECTURES

Plasmonics for biological applications based in interfacial self-assembly

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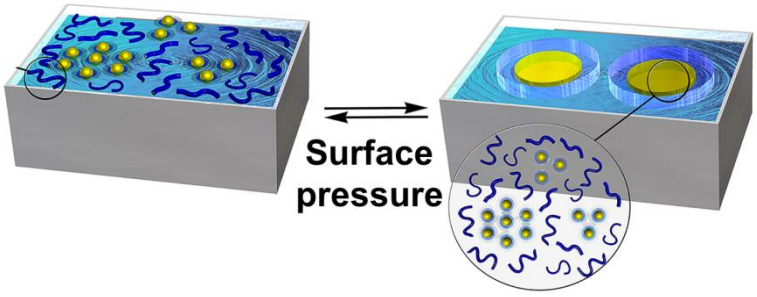
The incorporation of plasmonic nanoparticles in Langmuir monolayers appears as a stimulant and fruitful field of research.[1] The fine control of the assembling processes and applied surface pressure provided by the Langmuir technique provides highly attractive conditions to form well-defined supramolecular structures of plasmonic nanoparticles.

The assembled plasmonic structures can be used in a number of biological applications. Two avenues of research are considered herein. First, the actuation on different biomaterials through the functionality of the plasmonic structures. Second, the mimicking of simple biological entities related with early life forms.

Exploiting the localized surface plasmon resonance activated by a remote source of light, eukaryotic cells could be seeded and grown on plasmonic structures, being subsequently retrieved by laser irradiation. The plasmonic nanoparticles in this case provide not only the plasmonic field, but also a readily available Au surface that can be easily functionalized with any given biomolecule of interest.[2]

Plasmonic nanoparticles also serve as excellent building blocks for assembling supramolecular structures that mimic biological behaviour. We have explored mechanosensation, i. e., conversion of applied pressure to defined modification in molecular arrangements. This feature has been achieved through hybridization of the nanoparticles with a purposefully designed self-assembling molecule based on non-covalent intermolecular interactions.[3]



Cooperative self-assembly of gold nanoparticles at the air/liquid interface

Acknowledgements
J.J.G.-C. acknowledges the Ministry of Economy and Competitiveness for a Ramón y Cajal contract(#RyC-2014-14956).

References
[1] J. J. Giner-Casares, G. Brezesinski, H. Möhwald, Curr. Opin. Colloid Interface Sci., 19 (2014) 176.
[2] J. J. Giner-Casares, M. Henriksen, I. García, L. Liz-Marzán, Angew. Chem. Int. Ed., 55 (2016) 974.
[3] J. P. Coelho, M. J. Mayoral, L. Camacho, M. T. Martín-Romero, G. Tardajos, I. López-Montero, E. Sanz, D. Ávila-Brande, J. J. Giner-Casares, G. Fernández, A. Guerrero-Martínez, J. Am. Chem. Soc., 139 (2017) 1120.

Synthesis and Optical Studies of Silica Encapsulated Quantum Dots During Optical Trapping

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SiO_2encapsulation of colloidal quantum dots (QDs) shows differences in terms of optical properties and luminescence quantum yield, depending on the surface composition, size, and ligand content. In this work, emphasis has been placed on the fine control required to obtain luminescent SiO_2 encapsulated QDs by studying the role of different ligands by means of XPS and NMR (including DOSY and NOESY) spectroscopies. [1]. Furthermore, optical trapping [2,3] of these encapsulated QDs allows for their manipulation and acquisition of their optical properties and evolution in solution. In particular, the trade-off between photo-brightening and photo-bleaching controlling their emission stability will be discussed.The results emphasize the importance of surface chemistry in colloidal QDs, especially for imaging applications in polar liquid media.

Acknowledgements
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References
[1] M.Acebrón et al. ACS Appl. Mater. Interfaces, 7 (2015) 6935–6945.
[2] S. Hormeño et al. Nano Lett., 11 (2011) 4742-4747.
[3] S. Hormeño et al. Small, 10 (2014) 376-384.

Role of counter-ion and helper lipid content in the design and properties of nanocarrier systems: a biophysical and biological study

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Liposomes composed of MO and cationic lipids from the dioctadecyldimethylammonium family (DODAX, where X stands for Br- or Cl-) have shown to be efficient nucleic acid delivery systems and proteins [1,2]. Dioctadecyldimethylammonium bromide (DODAB) and chloride (DODAC) assemble into bilayer structures when dispersed in aqueous media above the phase transition temperature [3]. Although only differing in the counter-ion, they form vesicles that after conjugation with nucleic acids originate lipoplexes with different characteristics. Indeed, DODAB:MO and DODAC:MO lipoplexes were tested for gene delivery purposes and compared in terms of gene knockdown, toxicity, and stability in human serum [4]. There is a direct correlation between the physicochemical properties of nanocarrier systems and their biological performance, including stability under physiological conditions, cellular internalization and transfection efficiency. Therefore, understanding the biophysical aspects that affect self-assembled nanocarriers is determinant for a rational design of efficient formulations. In this study, a comprehensive evaluation of the effects of each component on the molecular organization of aggregates formed by the cationic lipids dioctadecyldimethylammonium bromide and chloride (DODAB and DODAC) and the neutral lipid monoolein (MO) was made. Specifically, the effects of the helper lipid content (MO) and the role of the counter-ion of the cationic lipids were evaluated in 2D and 3D assemblies by Langmuir surface pressure–molecular area (π–A) isotherms, Brewster Angle Microscopy (BAM), infrared reflection absorption spectroscopy (IRRAS), confocal Raman microscopy, and Small Angle X-ray Scattering (SAXS). The results show that MO has a different distribution on the DODAC and DODAB bilayers, and a fluidizing effect dependent on the MO content. For low MO molar ratios, the fluidizing effect was more pronounced in DODAC:MO mixtures, indicating a more homogeneous distribution of MO in DODAC than in DODAB bilayers. For high MO molar ratios, packing of membranes was similar for both cationic lipids, and the effect of the counter-ion is attenuated. The distribution of MO in the two cationic systems is closely related with the efficiency of the counter-ions in the screening of the charged group. Important effects on liposome properties of the counter-ions and MO content were observed, affecting cellular internalization, silencing of eGFP protein expression and overall cytotoxicity in different cell lines.

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References
[1] J. P. Silva, A. C. Oliveira, M. Lucio, A. C. Gomes, P. J. Coutinho and M. E. Oliveira, Colloids Surf., B, 2014, 121, 371–379.
[2] C. Carneiro, A. Correia, T. Collins, M. Vilanova, C. Pais, A. C. Gomes, M. E. Real Oliveira and P. Sampaio, Eur. J. Pharm. Biopharm., 2015, 89, 190–200.
[3] E. Feitosa and F. R. Alves, Chem. Phys. Lipids, 2008, 156, 13–16.
[4] A. C. Oliveira, T. F. Martens, K. Raemdonck, R. D. Adati, E. Feitosa, C. Botelho, A. C. Gomes, K. Braeckmans and M. E. Real Oliveira, ACS Appl. Mater. Interfaces, 2014, 6, 6977–6989.

IESMAT: Scientific instrumentation for Characterization of COLLOIDS

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The presentation will deal with different technologies for colloids characterization, among them:
-Laser diffraction-DIF: Particle size in the micron range (Mastersize, Malvern Instruments).
-Dynamic Light Scatteting-DLS/M3-PALS (Malvern Instruments): Particle size and ζ potential of particles with size in the nanometer scale.
-Nanoparticles Tracking Analysis-NTA (Malvern Instruments): Determination of the particle size and the particle concentration.
-REO: Rotational rheology (MalvernInstruments)
-DWS (Multi-Speckle Diffusing Wave Spectroscopy):Optical rheology. Formulation.
-Microfluidic rheology: high shear rheology. Formulation.
-Multiple Light Scattering-MLS: Stability of emulsions, suspensions, foams.Formulation.
-Microfluidic: High shear processing.Size decrease, encapsulation.Microfluidics.
-FFF-Field Flow Fractionation: Separation, particle fractioning.

From macroscopic molecular gels to molecular nanoparticles for transport and delivery of actives

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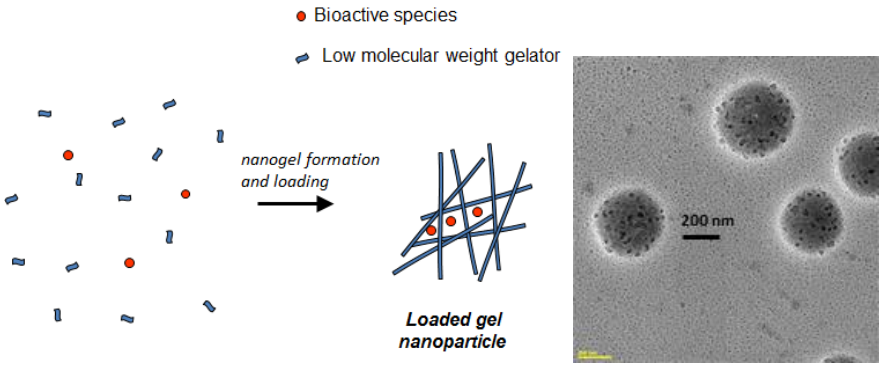
Molecular gels, as opposed to polymeric ones, are composed of low molecular weight species. Supramolecular 1-D assembly of molecular gelators affords fibrillary microstructures that percolate the solvent and afford self-sustained gels. [1, 2] This type of soft materials have attracted increasing attention due to some advantages associated to their non-covalent and intrinsic reversible nature such as stimuli responsiveness, biocompatibility and biodegradation.[3] Applications of molecular gels have blossomed in the last decade in different areas such optoelectronics, catalysis, controlled release or tissue engineering.[4]
Here we report on our recent findings in the use of low molecular weight gelators as building blocks for nanoparticles with envisaged applications in biomedical issues related to drug delivery and sensing. Molecular nanoparticles (nanogels) might represent an interesting alternative of polymeric analogues used in Nanomedicine. Four different approaches for nanogel preparation are presented: ultrasonication, controlled precipitation, use of liposomes as template and microfluidics. The nanomaterials are characterized by dynamic light scattering, electron microscopy and fluorescence. Additionally, their kinetic and thermodynamic stability is evaluated. The capability of the nanoparticles to be loaded with different photoactive units and evaluation of their intracellular delivery capabilities will also be discussed.



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References
[1] R. G. Weiss, J. Am. Chem. Soc., 136, (2014), 7519-7530.
[2] A. R. Hirst, I. A. Coates, T. R. Boucheteau, J. F. Miravet, B. Escuder, V. Castelletto, I. W. Hamley and D. K. Smith, J. Am. Chem. Soc., 130, (2008), 9113-9121.
[3] M. D. Segarra-Maset, V. J. Nebot, J. F. Miravet and B. Escuder, Chem. Soc. Rev., 42, (2013), 7086-7098.
[4] A. R. Hirst, B. Escuder, J. F. Miravet and D. K. Smith, Angew. Chem. Int. Ed., 47, (2008), 8002-8018.

Lipid nanosystems for therapeutic purposes – biophysical studies as useful tools to understand interactions at the nano–bio interface

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To achieve optimal therapeutic results, drug delivery systems in general and controlled release nanosystems in particular should be designed taking into account various aspects such as: the biological barriers encountered by the nanosystem; its route of administration; its absorption, distribution, metabolism and elimination; its target tissue and its selective toxicity [1].

In this lecture, the development of drug delivery nanosystems is presented as a rational sequence of steps taking into account the therapeutic target and the active compound, as well as the biological interfaces. These are extremely important factors to consider in the design of nanosystems and are usually evaluated only at a later stage of formulation development.

A series of biophysical studies are presented as tools to evaluate either interactions between drug and the nanosystem or interactions between drug and the bio-interfaces or even between the nanosystems and some bio-interfaces. These *in vitro* biophysical studies are not surrogates of *in vivo* studies but can be very useful for screening the most promising formulations and to early identify problems during formulation development at an early stage.

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References
[1] M. Lúcio, J. L. F. C. Lima and S. Reis, *Drug-membrane interactions: Molecular mechanisms underlying therapeutic and toxic effects of drugs* in *Ideas in Chemistry and Molecular Sciences*. Pignataro, Bruno (ed.) March 2010. Wiley-VCH, Weinheim ISBN-13: 978-3-527-32541-2. [DOI: 10.1002/9783527630516.ch8]

Surface modification with functional alkoxysilanes: a valuable route for selective and effective magnetic nanosorbents

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Magnetic nanomaterials are very attractive for separation processes because besides bearing a large surface area that favors adsorption, the magnetic features allow the easy magnetically assisted separation of target species from the surrounding medium. Surface functionalization plays a key role in the design of magnetic adsorbents.[1] The use of functional alkoxysilanes is one of the most common procedures for surface derivatization of magnetic iron oxides. Furthermore a wide variety of alkoxysilanes appeared commercially available in the last years, opening a range of novel opportunities in the surface derivatization of magnetic nanoparticles. Nevertheless further research is needed to develop more effective magnetic nanosorbents, namely through the optimization of the functionalization of nanomaterials surface for maximizing selectivity, sorption capacity and reuse.

Herein we report the preparation of magnetic nanosorbents for two distinct applications, water treatment and protein enrichment, using functional alkoxysilanes for the functionalization of surfaces sorbents. Following this synthesis approach, magnetic nanoparticles with metal ion chelating moieties grafted on their surface enabled to selectively recover metalloproteases even in highly diluted saliva samples via magnetic separation. These materials were proven to be valuable probes for the selective enrichment and rapid recovery of metalloproteases from human saliva, a complex matrix, particularly when dealing with trace amounts of material. [2] In another system, an alkoxysilane containing isocyanate groups was used to grow hybrid siliceous shells enriched in polysaccharides covalently bonded to magnetite surfaces', as a strategy to develop low cost, eco-friendly nanosorbents for water treatment [3]. This method led to magnetic nanosorbents that exhibited very high adsorption capacity over consecutive adsorption/desorption cycles, which demonstrates the reusability potential and robustness of these hybrid sorbents.

Acknowledgements
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References
[1] K. Hola, Z. Markova, G. Zoppellaro, J. Tucek and R. Zboril, Biotech. Adv. 33 (2015) 1162-1176.
[2] R. Oliveira-Silva, J. Pinto-da-Costa, R. Vitorino and A. L. Daniel-da-Silva, J. Mater. Chem. B, 3 (2015) 238-249.
[3] S. F. Soares, T. R. Simões, M. António, T. Trindade and A. L. Daniel-da-Silva, Chem. Eng. J., 302 (2016) 560–569.

Multilayered and 3D structures of Bacterial cellulose composites with nanoparticles

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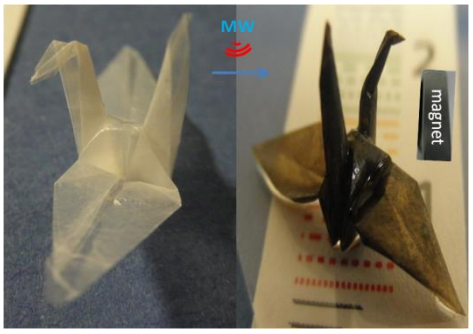
Cellulose constitutes an almost inexhaustible biopolymer, being the most abundant renewable polysaccharide produced in the biosphere. Cellulose is predominantly obtained from plants; however it can also be synthesized by bacteria, algae and fungi. In particular, cellulose obtained by bacteria has the same molecular formula as vegetal cellulose but exhibits a high degree of polymerization, crystallinity and, importantly, does not contain lignin and hemicelluloses, increasing its biocompatibility. We can obtain bacterial cellulose (BC) films characterized by a three-dimensional architecture of cellulose fibers forming an interconnected open pore network. BC films also have high porosity, transparency in the UV-NIR and a high water holding capacity. The bacterial synthesis of BC allows us to control the micro(nano)structuration, 3D structure and shape of the BC materials.

Industries, governments and consumers appeal for the use of green, sustainable and natural resources for the fabrication of advanced complex materials. Thus, the biosynthesized cellulose emerges as a highly interesting bio-polymer to study structure, topography and new bottom up approaches to fabricate novel nanocomposites.

We will present the production and characterization of cellulose films and the impact that different physical and chemical parameters such as the bacterial culture properties, drying method and chemical modification have on its microstructure, porosity, wettability, transparency and mechanical properties. Additionally, I will also present the modification of BC with different inorganic nanocrystals which allows us to obtain value-added engineered nanocomposites responsive to different stimuli. These innovative bacterial cellulose structures will provide the proof of concept for devices or products.



References

[1] Zeng et al. Journal of Materials Chemistry C 2 (2014) 6312-6318 DOI: 10.1039/c4tc00787e
[2] Zeng et al. Cellulose (2014) 21 4455–4469 DOI 10.1007/s10570-014-0408-y

ORAL COMMUNICATIONS

TOPIC 1: NANOPARTICLES

Copper sulfice nanocrystals@graphene: synthesis and photocatalytic activity

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Semiconductor nanocrystals (NCs) have been extensively explored due to their unique size dependent optical and electronic properties, which are of interest in a number of applications including photocatalysis [1]. In particular,copper sulfide has been investigated as a photocatalyst of interest due to the ability to harvest photons efficiently in the visible spectral region, exhibiting a band-gap (Eg=1.2-2.2 eV), which is dependent on the crystalline phase present [2]. On the other hand graphene based materials have also attracted great importance due to their unique properties [3]. The implementation of chemical routes aiming to combine these two types of materials opens new routes for the development of innovative nanodevices. For example, the combination of graphene oxide with copper sulphide materials has been reported as a promising strategy for the development of hybrid photocatalysts [4]. In this context, we have investigated the *in situ* growth of copper sulphide ($Cu_{2-x}S$) nanocrystals, in the presence of graphene oxide (GO) flakes dispersed in ethanol, by the sonolytic degradation of dissolved Cu(II) dialkyldithiocarbamate complexes. The new materials were firstly tested as photocatalysts using a visible light photoreactor and an organic dye as the water contaminant model. The photocatalytic activity of the hybrid photocatalysts will be discussed on the basis of relevant literature, namely by putting in perspective their application in the photodegradation of emergent pollutants such as pharmaceutical compounds dissolved in water.

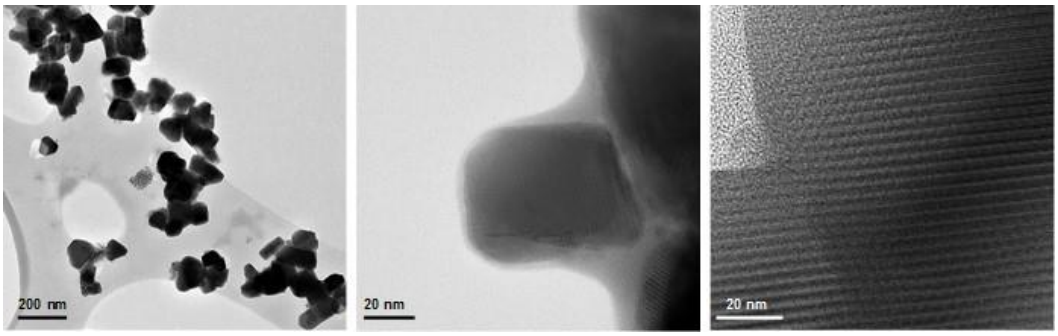

Fig. 1 TEM images of copper sulfide nanocrystals with rhombohedral structure.

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References

[1] T. Trindade and P. J. Thomas in *Comprehensive Inorganic Chemistry II: From Elements to Applications* (Eds.: J. Reedijk and K. Poeppelmeter), Elsevier, Oxford, 2013, 4, 343-369.
[2] (a) R. K. Upadhyay, N. Soin and S. S. Roy, RSC Adv., 4 (2014) 3823-3851; (b) A. C. Estrada, F. M. Silva, S. F. Soares, J. A. P. Coutinho and T. Trindade, RSC Adv., 6 (2016) 34521-34528.
[3] Y. Zhao, H. Pan, Y. Lou, X. Qiu, J. Zhu and C. Burda, J. Am. Chem. Soc., 131 (2009) 4253-4261.
[4] (a) Y. Wang, L. Zhang, H. Jiu, N. Li, and Y. Sun, Appl. Surf. Sci., 303 (2014) 54-60; (b). M. Saranya, R. Ramachandran, P. Kollu, S. K. Jeong and A. N. Grace, RSC Adv., 5 (2015) 15831-15840.

Synthesis, characterization and evaluation of magnetic doped ferrites as potential therapeutic tools

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In last decades, magnetic nanoparticles (MNPs) have been intensively studied due to their potential technological and biomedical applications [1]. Many of the synthetic techniques used to obtain magnetic nanoparticles have serious limitations in terms of costs and versatility, being thermal decomposition[2] one of the most robust and reproducible methods to obtain nanoparticles with a high purity and crystallinity while simultaneously achieving a great control over their shape and size. This work presents the synthesis and characterization of MNPs obtained by thermal decomposition with different metallic compositions. We analyzed the influence of molar ratios between iron, manganese, cobalt and zinc precursors and different parameters of the synthetic process on MNPs formation, structure and physical properties. In this manner, we have achieved an optimization of the synthetic process of doped MNPs with full control over their composition, size and magnetic properties in order to choose those particles with best hyperthermia and contrast imaging properties for biomedical applications. The oleic acid-oleylamine capped MNPs were transferred to aqueous solution via an *in situ* polymer coating process with dodecylamine-grafted poly(isobutylene-alt-maleic anhydride) (PMA) [3] in order to check their potential cytotoxicity, cellular uptake profiles and therapeutic capabilities *in vitro* in different cell lines.

Acknowledgements
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References
[1] N. Lee, D. Yoo, D. Ling, M. Cho, T. Hyeon, J. Cheon, Chem. Rev., 115 (2015) 10637-10689
[2] D. Ling, N. Lee, T. Hyeon, Acc. Chem. Res., 48 (2015) 1276-1285.
[3] Q. Zhang, I. Castellanos-rubio, R. Munshi, I. Orue, B. Pelaz, K. I. Gries, W. J. Parak, P. del Pino, A. Pralle, Chem. Mater. 27 (2015) 7380-7387.

Raman imaging for the investigation of antimicrobial fabric dyeing

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There has been great interest from the textile industry on the production of fabrics loaded with nanoparticles (NPs) in order to confer new properties to conventional products.[1,2] New functionalities that arise from the incorporation of metallic NPs on textile fibers make them good candidates in domains such as wound dressing, smart textiles and biosensors.[1,2] In particular, textile fibers doped with Ag NPs have been explored due to their antimicrobial properties.[3] This communication highlights the relevance of new available Raman spectroscopic methods to monitorthe dyeing process in antimicrobial textiles, which is a critical stage in the manufacture process of fabrics.[4] This approach takes advantage on the presence of Ag NPs in the fibers to monitor the adsorption of the organic dyes on the metal surfaces and, on the other hand, to probe the location of the Ag NPs over the fibres. This possibility arises due to surface enhanced Raman resonance scattering (SERRS) effects coming from the organic dye adsorbed at the Ag NPs. Hence, linen fibers loaded with Ag NPs and then stained with methylene blue (MB) were used as working systems to exploit this new characterization protocol. MB was selected as the molecular probe not only because is a common organic dye but also it occurs in the form of dimer or monomer species each with characteristic visible absorption and Raman spectra. It will be demonstrated that the SERRS effect together with confocal Raman microscopy offer a new tool to map the local distribution of the MB dye in the fibers by Raman imaging and consequently the distribution of Ag NPs over the fabrics. In addition, it is also possible to assess the preferred adsorbate form of MB on distinct types of nanocomposite fibers and their local distribution.[5] This investigation allows to foreseeing the use of this approach in terms of quality control of antimicrobial Ag containing fabrics, which is a market in great expansion.

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References
[1] R. Dastjerdi, M. Montazer, Colloids Surfaces B Biointerfaces, 79 (2010) 5
[2] R. J. B. Pinto, M. C. Neves, C. P. Neto, and T. Trindade, "Composites of Cellulose and Metal Nanoparticles," in Nanocomposites - New Trends and Developments, (2012) 73.
[3] P. J. Rivero, A. Urrutia, J. Goicoeche, F. J. Arregui, Nanoscale Res. Lett. 10, (2015) 501
[4] S. Fateixa, M. Wilhelm, H. I. S. Nogueira, T. Trindade, J. Raman Spectrosc., 47, (2016) 1239
[5] S. Fateixa, M. Wilhelm, A. M. Jorge, H. I. S. Nogueira, T. Trindade, J. Raman Spectrosc., (2017)

Versatile magnetic biohybrid nanosorbents for the removal of herbicides from water

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Since their introduction in the 1940s, the chemical herbicides have been of great importance in the modern agriculture by providing a very efficient way of controlling weeds in farming areas.Nevertheless, the misuse of some widely-used herbicides, e.g. glyphosate and paraquat, resulted in their environmental accumulation and in the contamination of water sources[1,2]. Due to their negative impact on environment and human health[3-5], there is an urgent need to develop effective methods for water remediation contaminated with these herbicides. Magnetic nanomaterials are very attractive as sorbents because besides bearing a large surface area that favors adsorption, possess magnetic features that allow the easy magnetically assisted separation from the treated water.

This work presents the synthesis and characterization of novel magnetic hybrid nanosorbents and the performance towards the removal of herbicides from water [6]. These materials are composed of a magnetite core, protected with a hybrid siliceous shell containingbiopolymers covalently linked. Based on this approach, four hybrid materials were prepared with the polysaccharides κ-carrageenan, starch (rice), chitosan and quaternary ammonium chitosan (HTCC) respectively. By introducing polysaccharides with distinct chemical nature, it was possible to obtain hybrid materials of variable surface chemistries. In addition, for the first time, magnetic nanosorbents functionalized with biopolymers were efficiently employed for the remediation of water contaminated with herbicides. For example, it was found that the hybrid particles prepared from κ-carrageenan and HTCC exhibit the highest performance for paraquat and glyphosate removal, respectively. As such, these materials have been investigated in the uptake of these herbicides from water using variable operational conditions, namely at distinct pH, herbicide concentration and contact time.Besides the high adsorption capacity, the clean-up could be easily achieved with a magnetic gradient and the particles recycled by ion exchange while keepingtheir performance for several cycles.

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References
[1] Ikpesu, T.O. *Environ. Sci. Pollut. Res.* **2015**, *22*, 8517-8525 (10.1007/s11356-014-3993-2).
[2]Casida, J.E.; Durkin, K.A. *Chem. Res. Toxicol.***2017**, *30*, 94-104. (10.1021/acs.chemrestox.6b00303).
[3]Tsai, W.T. *Toxicol. Environ. Chem.* **2013**, 95, 197-206 (10.1080/02772248.2012.761999).
[4] Myers, J.P.; Antoniou, M.N.; Blumberg, B.; Carroll, L.; Colborn, T.; Everett, L.G.; Hansen, M.; Landrigan, P.J.; Lanphear, B.P.; Mesnage, R., *et al.Environ. Health* **2016**, *15*, 19, (10.1186/s12940-016-0117-0).
[5] Bai, S.H.; Ogbourne, S.M. *Environ. Sci. Pollut. Res.* **2016**, *23*, 18988-19001 (10.1007/s11356-016-7425-3).
[6] Fernandes, T.; Soares, S.; Trindade, T.; Daniel-da-Silva, A.L. *Nanomaterials***2017**, *7*, 68 (10.3390/nano7030068)

Oral **O-5**

Gold-based hybrid nanoplatforms as tools for oncogenic pathway inhibition of aggressive tumors through a combinatorial multi-therapeutic approach.

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The human epidermal growth factor receptor (HER) family of tyrosine kinases is deregulated in multiple cancers either through amplification, over-expression, or mutation, causing its carcinogenic effect [1]. HER3 and HER2 oncogenes are commonly over-expressed in the most aggressive forms of cancer. In particular, HER3 amplification is present in breast, colon and gastric tumors [1], and a high expression is positively associated with the presence of lymph node metastases [2]. In addition, HER2 has been found in approximately 30% of human breast cancers and shown to render cancer cells more resistant to chemotherapy [3]. However, the mutant HER3 oncogenic activity is dependent on HER2 signaling [1]. Expression of HER2 alone does not significantly enhance drug resistance, which is related to other HERreceptors like HER3 [4]. In recent studies, HER2 has been found highly phosphorylated in cells coexpressing at the same time HER2 with HER3, as for NIH 3T3 or SKBR3 cells [4] Thus, HER3 presence may be correlated with bioresponses to chemo-treatments that target HER2, providing a route for resistance to anti-HER drugs and drug targeting strategies [3]

Oncogenic tyrosine kinases have proven to be promising targets for the development of highly effective anticancer drugs [5]. Some studies have shown the benefits of an effective combinatorial treatment using anti-HER antibodies with small molecule inhibitors which effectively blocks mutant HER3 [1]. Herein, we propose a nanoplataform with multitherapeutic capability against HER2 and HER3 receptors. This nanocarrier consist of a hybrid gold nanoshell functionalized with the antibody Trastuzumab and a silencing RNA (siRNA) against HER3. We observed that HER3, HER2 and, consequently, the PI3K/Akt signaling route are inhibited in SKBR3 cells (positive HER 3 and HER2 cells) and MDA-MB-231 cells (only HER2 positive) in vitro, noting that HER3 knocking down involves the induction of of cell apoptosis and subsequent death.

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References

[1] B. S. Jaiswal, N. M. Kljavin, E. W. Stawski, E. Chan, C. Parikh, S. Durinck, F. J. de Sauvage, Cancer Cell, 23 (2013) 603-617.

[2] N. R. Lemoine, D. M: Barnes, D. P. Hollywood, C. M: Hughes, P. Smith, E. Dublin, S. A. Prigent, W. J. Gullick, H. C. Hurst, J. Cancer, 66 (1992) 1116-1121.

[3] C. Desbois-Mouthon, Gastroenterologie Clinique et Biologique, 34 (2010) 255-259.

[4] C. Xhen, T. K. Yeung, Z. Wang, Biochem. Biophys. Res. Commun., 277 (2010) 757-763.

[5] N. V. sergina, M. Rausch, D. Wang, J. Blair, B. Hann, K. M. Shokat, M. M. Moasser, Nature, 445 (2007)437-444.

Oral **O-6**

A problem with solution: Development of lipid-based colloidal nanocarriers for encapsulation of compounds with weak bioavailability

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Curcumin, the golden powder with weak bioavailability, also known for its anti-inflammatory and antioxidant properties, has been a target of great heed in various medical fields, namely in the treatment of neurodegenerative diseases [1]. In this particular field, multiple pharmacological targets, capable of promoting a decrease in peptidic aggregation [2], [3], oxidative stress [4] and neuroinflammation [5] have been identified.

Considering that the level of biomedical activity is highly dependent on the proportion of curcuminoids, a prior study of the pharmaceutical profile of *C.longa*, the biggest source of curcuminoids, of *C. aromatica*, known for its medical relevance, and commercial curcumin, whose chemical constitution is known, was conducted [6]. This initial study was based in *in vitro* studies using a toolbox of biophysical techniques: derivative spectroscopy; quenching of intrinsic fluorescence of human serum albumin; dynamic and electrophoretic light scattering, differential scanning calorimetry and small and wide angle x-ray diffraction. The results obtained revealed that the studied bioactives possess low bioavailability, low solubility, fast breakdown, bioaccumulation, high affinity to HSA, membrane biophysical impairment and highlighted the need of encapsulating curcumin and extracts using nanocarriers.

Following this rationale, and in order to optimize the use of such compounds in the treatment of neurodegenerative diseases, this research is focused on encapsulating curcumin and both the *C. longa* and *C. aromatica* extracts, in lipid-based colloidal nanosystems of dioctadecyldimethylammonium bromide (DODAB) and 1-oleoyl-*rac*-glycerol (MO) (1:2).

The nanocarriers obtained by ethanolic injection of the bioactives in the nanosystems showed an encapsulation efficiency of approximately 100 %, being, thereby, highly efficient at encapsulating curcumin and extracts. Additionally, the same nanocarriers exhibited sizes inferior to 200 nm, high stability when stored up to 4 months and a positive superficial charge, which constitute attractive features for biomedical applications. A high affinity of curcumin and the studied extracts to the liposomes, as well as the ability to prevent interactions with plasma proteins, after successful pegylation, was also confirmed. As final remark, the formulations developed herein confirmed the antioxidant activity of the encapsulated natural compounds.

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Hybrid nanoparticles for oral drug administration

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Nanostructured lipid carriers (NLC) are nanosystems (40-1000 nm) considered a second and smart generation of lipid nanoparticles, consisting of a matrix composed of a blend of solid and liquid lipids (oils), stabilized by an aqueous emulsifier solution [1]. This type of lipid nanoparticles has shown interesting properties (smallsize, large surface area, high drug loading, biocompatible and biodegradable nature, control over drug release, etc), that allow their use as drug nanocarriers. Polymer coating of NLC has provided an improved performance in drug delivery, arising as an appealing technological option [2].

The aim of this work was the development of hybrid polymer-lipid nanoparticles, with chitosan as the polymer, for oral administration of carbamazepine (CBZ).CBZ is a first-line drug for the treatment of epilepsy in spite of its variable absorption and high first-pass effect mediated by the isoform CYP3A4. Chitosan, a biopolymer with mucoadhesion properties,was chosen for coating, because it is reported to decrease particle aggregation in acidic medium and promote mucoadhesion [3], leading to a controlled drug release and improved bioavailability.

Hybrid nanoparticles were produced by the hot high pressure homogenization technique and were evaluated in terms of physicochemical properties,*in vitro* release, intestinal permeability, and *in vivo* performance.

Optimized hybrid nanoparticle formulation presented a particle size of 178 ± 32 nm,along with a polydispersity index of 0.241 and a zeta potential of 38 ± 11 mV. The*in vitro* release profiles suggest a controlled release of CBZ, due to the chitosan coating. Permeability and *in vivo* studies support the release behaviour, also indicatingthat higher concentrations of CBZ were obtained in the brain tissue when the drug was incorporated within hybrid nanoparticles in relation to those achieved with CBZ in suspension.

In this way, the hybrid chitosan lipid nanoparticles formulation has shown advantages in opposition to the conventional lipid nanoparticles, and the commercial oral solution, being considered a good candidate to encapsulate CBZ and improve its therapeutic efficacy in the treatment of epilepsy.

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References

[1] C. Vitorino, J. Almeida, L.M. Gonçalves, A.J. Almeida, J.J. Sousa, A.A.C.C. Pais, J Control Release, 167 (3) (2013), 301-314.

[2] M. Mendes, H.T. Soares, L.G. Arnaut, J.J.Sousa, A.A.C.C. Pais, C. Vitorino. Int J Pharm, 515 (1–2) (2016) 69-83.

[3] Y. Luo, Z. Teng, Y. Li, Q. Wang. *Carbohydr Polym*, 122 (2015) 221–229

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Development of lipid-based colloidal nanocarriers for topical application of acyclovir

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Herpes infections are very frequent infectious diseases, especially in individuals whose immune system is weakened, causing manifestations in the central nervous system that leave severe squeals in about 80% of cases. There are several types of etiologic agents of herpes infections, the most famous being the Herpes Simplex Virus HSV 1 and 2. HSV 1 usually affects the face, lips, gums, palate, tongue and nasal mucosa and can spread to other parts of the body and HSV 2 reaches the genital area, affecting both men and women [1].
The most common current therapies to treat herpes infections are based on topical application of creams containing an antiviral agent, but whose effectiveness is limited due to low skin penetration of the active agent , thus requiring the application of about four or up to five times per day for improving the therapeutic effectiveness of the formulation [1]. For this reason , there is great interest in developing formulations based on the use of nanocarriers of active ingredients to promote more effective penetration through the skin and thus to reduce the frequency of application.
Biophysical characterization of the most common drug used to treat herpes, acyclovir, also revealed some pharmacokinetic problems related with drug biodistribution accessed by determination of: (i) distribution coefficients in membrane/water systems by derivative spectrophotometry; (ii) binding constants of the drug to serum human albumin by fluorescence quenching, dynamic and electrophoretic light scattering and (iii) drug effect on membrane microviscosity accessed by dynamic light scattering.
To overcome the biodistribution problems found for acyclovir, this work further proposes the development of nanostructured lipid carriers (NLC) and monoolein based colloidal carriers containing the anti-viral drug. Formulations were evaluated regarding their stability characteristics (size, polydispersity, surface potential and lipid phase transition properties), as well as, the drug encapsulation efficiency and their release profiles when in contact with the skin pH.
Finally, after selecting the formulation with the best biophysical characteristics, it was included in a vehicle (hydrogel) for topical application and the effects of the formulation on the rheological characteristics of the vehicle were evaluated to optimize the formulation with improved galenic properties. After the incorporation of the nanocarriers in the hydrogel it has demonstrated a pseudoplastic behavior with thixotropy favoring its administration.

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References
[1] C. M. Lopes, J. Silva, M. E. C. D. Real Oliveira and M. Lúcio Lipid-based colloidal carriers for topical application of antiviral drugs, in Pharmaceutical Nanotechnology, volume III, Elsevier, 2017, *in press*

Miniemulsion polymerization as a synthetic platform for structure control of multifunctional polymer/metal oxide hybrid nanoparticles

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Hybrid polymer/inorganic nanoparticles have become popular in the last two decades. The integration of functionalities provided by inorganic components (e.g., optical, magnetic, electrical, catalytic functions) with the stability, processability, and biocompatibility properties of polymers allows for shaping complex nanomaterials with great applicability in a wide range of sectors. The combination of different inorganic functionalities within a polymer matrix acting as supporting material, nanocontainer or nanocarrier opens new possibilites towards the development of a second generation of more complex multifunctional hybrid nanoparticles. The specific location of the functional units has a key role in the properties of the final material, and its relevance increases with the complexity of the system. In this context, a deep understanding and a precise control over the morphological development of the hybrid nanoparticles is still a challenge.

The preparation of hybrid nanoparticles can be reached by different strategies, including electrostatic interactions (e.g., layer-by-layer deposition), covalent bonding or in situ preparation of the components [1]. This work establishes miniemulsion polymerization as a synthetic platform for the production of magnetically separable nanoparticles with controlled structure and high performance in heterogeneous catalysis. Magnetoresponsive (Fe3O4) and catalytically active (TiO2 or CeO2) metal oxide nanoparticles, produced either ex situ or crystallized in situ, are incorporated within a supporting matrix of poly(methyl methacrylate) (PMMA) or polystyrene. A schema of the general process is presented in Figure 1(a).

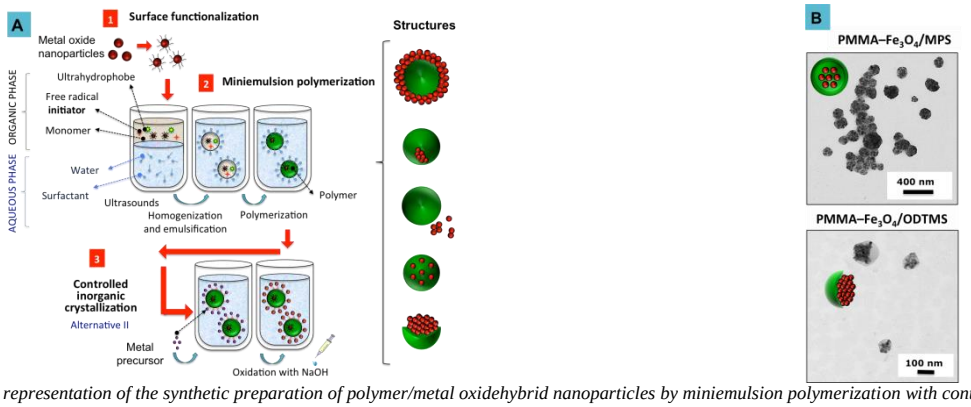

Fig. 1. (a) *Schematic representation of the synthetic preparation of polymer/metal oxidehybrid nanoparticles by miniemulsion polymerization with controlled structure. (b) Influence of the inorganic surface functionalization over the morphology of the hybrid system.*

The inorganic nanoparticles are first hydrophobized by usig silane chemistry for compatibilization with the monomer, which is polymerized afterwards by free radical polymerization in miniemulsion. A second generation of multifunctional particles results from the simultaneous incorporation of two inorganic species, whose final location will be determined by a self-assembly process driven by the minimization of the overall interfacial energies of the system [2]. An alternative approach was successfully developed by adding a post-polymerization step consisting of the controlled in situ crystallization of a second inorganic specie. The formation of an outer inorganic shell by complexation and further reduction of a metal oxide precursor requires the introduction of functional moieties (such as carboxylic groups) at the polymer surface by using a comonomer (e.g., acrylic acid) [3].

Miniemulsion polymerization is used to overcome the morphological restrictions of other colloidal techniques and to enable a complete inorganic encapsulation, the formation of core−shell, or even Janus structures. The selective migration of the inorganic components is addressed by tuning the surface hydrophobicity of the metal oxide nanoparticles using alkoxysilanes as functionalizing agents with different accessible functional groups and chain lengths. Figure 1(b) shows two examples of the influence of the coupling agent over the final morphology. The introduction of surface polymerizable moieties with 3-methacryloxypropyl trimethoxysilane (MPS) leads to a homogeneous distribution of the inorganic particles encapsulated within the polymer, while the presence of longer alkyl chains and the absence of polymerizable units in octadecyl trimethoxysilane (ODTMS) drive towards Janus-like structures [4,5]. The polarity of the initiator used to promote the polymerization process determines the mechanism of the reaction and the motion of the inorganic species within the forming polymer matrix [2]. Thus, the final hybrid morphology results from the combined effect of the relative polarity of the inorganic components and the initiator with respect to the monomer.

In conclusion, this work presents a versatile synthetic platform based on miniemulsion polymerizarion for the morphological control of polymer/metal oxide hybrid nanoparticles. We study the effect of the surface functionalization of the inorganic nanoparticles and the nature of the free radical initiator over the selective migration of the inorganic components. The strategy is further extended to a second generation of multifunctional magnetic nanoparticles with applicability in heterogeneous catalysis.

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References

[1] V. Fischer, M. B. Bannwarth, G. Jakob, K. Landfester, R. Muñoz-Espí. *J. Phys. Chem. C*, 117 (2013) 5999–6005.
[2] J. M. Asua. *Macromol. Chem. Phys.*, 215 (2014) 458–464.
[3] M. A. Hood, M. Mari, R. Muñoz-Espí. *Materials*, 7 (2014) 4057–4087.
[4] A. Schoth, E. S. Adurahim, M. A. Bahattab, K. Landfester, R. Muñoz-Espí. *Macromol. React. Eng.*, 10 (2016) 47–54.
[5] A. Schoth, A. D. Keith, K. Landfester, R. Muñoz-Espí. *RSC Advances*, 6 (2016) 53903-5391.

Oral **O-10**

Highly Controlled Synthesis of Gold Nanostars in Microdroplets

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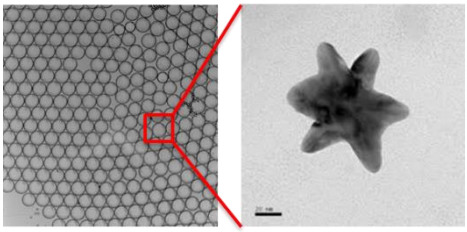
Synthesis of metallic nanoparticles, and ultimately of anisotropic metallic nanoparticles, has been a field of intense research in the past decade.[1] While controlling the composition of metal nanoparticles is fairly straightforward by the careful choice of the starting material, it is far more challenging when it comes to the control of their size and shape. This control over the morphology of the nanostructures is crucial for the desired applications and thus the optimization, control and reproducibility of synthetic procedures are to be pursued. The use of microfluidics as microreactors for the synthesis of nanomaterials has demonstrated to be successful in terms of reproducibility, homogeneity and automation.[2,3]Herein, we report on the monodisperse, reproducible, automatized and highly controllable synthesis of gold nanostars in a microdroplets platform. The monodispersity of the obtained material is comparable, if not better, to the corresponding synthesis in bulk, but more importantly, the process has been fully automatized by using the microdroplets technology. The possibility of the easy and rapid variation of reagent concentrations in the microdroplet environment led to a fine control over the size and number of spikes, and in consequence, over the optical and spectroscopic properties of the anisotropic material. A full characterization of the obtained samples proved the potential of this novel technology for the continuous synthesis of high quality gold nanostars. The technology presented here has a remarkable potential to be extended to different nanoparticle type synthesis, allowing for a better reproducibility and higher automation of protocols.



Acknowledgements

This work was supported by EU Framework Programme for Research and Innovation H2020 COFUND, Grant Agreement 713640 (SAC) and by FAPESP project No. 2015/01685-2 (PTB).

References

[1] Murphy, C. J. *et al.J. Phys. Chem. B*109, (2005) 13857–13870.

[2] Gomez, L. *et al.Lab Chip*14, (2014) 325–332.

[3] Abalde-Cela, S., *et al.Soft Matter*, 7 (2011) 1321-1325.

Crystal Engineering of Nano-Micro Particles in Polar Media

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Characteristics of functional nanomaterials are ultimately connected to their pathways of synthesis, which determine features such as their size, morphology, defects, surface protection, internal polarity and self-assembly behavior. Thus, functional properties depend on crystalline features, which in turn are rooted in the mother medium of reaction. An example particularly intriguing is the connection between the intrinsic polarity of nascent semiconductor nanocrystals and the polarity of the mother fluid in which they were grown.[1] Understanding of such an influence should allow access to crystal engineering of intricate shapes exhibiting novel functionalities and applications. Also, control over both self-assembly (SA) and its inevitable opposite disassembly or deconstruction should be achieved.

Here, we illustrate singular patterns of nanocrystal growth and deconstruction in highly polar reaction media through two case examples. As fluids of reaction, we chose ionic liquids and molten salts, which share special properties for the synthesis of nanoparticles: low surface tension, high viscosity, low melting temperature and large polarity and electrostatic contrasts [1]. In all the cases, the absence of long-change ligands eliminated their role in guiding the crystalline shape as well as in creating insulating organic barriers which are detrimental for electronic or catalytic applications.

First, we show the formation and deconstruction of star-like PbS hierarchical superstructures through five different stages corresponding to different SA patterns (Figure 1). Those are related to switches of polarity of the solvent and concomitant changes of intrinsic polarity of crystals as well as of electrostatic interactions [2]. Throughout all the stages, ubiquitous octahedral geometries account for the equilibration of dipolar forces in pairs of opposite direction along the vertexes of an imaginary octahedron. The critical role of polarization energy of the semiconductor crystals as self-limiting factor for SA is highlighted.

Second, we report the formation of octahedral NiO crystals with dimensions from the nano- to meso- and micro-scales (Figure 2). The maintenance of octahedral shapes in this face-centered cubic (fcc) structure is related to the stabilization of eight charged {111} faces in highly ionic medium provided by a mixture of hydroxides. We propose that the different sizes across varied length scales are obtained as a function of the degree of polarity of the reaction media in each case. Using this knowledge, one can realize controlled crystal engineering of polar crystals.

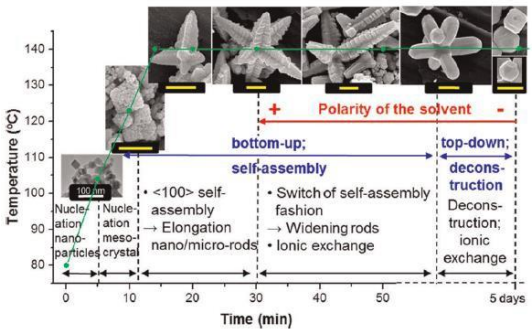

Figure 1. Temperature profile of reaction mixture (green line) containing ionic urea/choline chloride deep eutectic solvent and PbS nano/microstructures. TEM or SEM images of the PbS products at different reaction times. Scale bars are 500 nm except for the image at tr = 5 min.

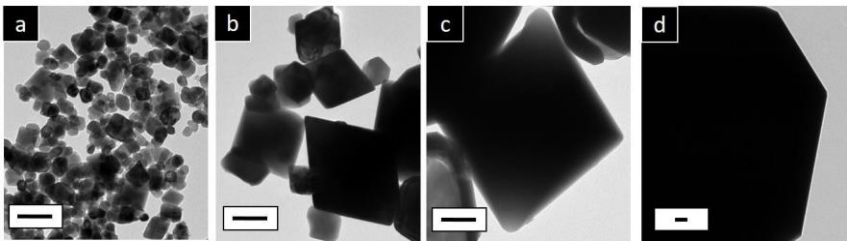

Figure 2. NiO octahedral (a-b) nanoparticles, (c) sub-micron particles and (d) microparticles obtained in molten NaOH/KOH mixture under different conditions: (a) without and (b-d) under autogenerated pressure; and with (a-b) 0, (c) 2 and (d) 12 mL of water. Scale bars are 100 nm.

Acknowledgements

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References

[1] Ana Querejeta Fernández. New Strategies for the Synthesis of Nanostructured Inorganic Functional Materials. Universidad Complutense de Madrid , Servicio de Publicaciones **(2011).**

[2] Querejeta-Fernández, A. *et al.* Unknown Aspects of Self-Assembly of PbS Microscale Superstructures. ACS Nano **(2012)** 6, 3800-3812.

Drug biophysical profiling using lipid-based colloidal nanosystems and human serum albumin as biomimetic interfaces

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The development of new drugs is a highly complex and expensive process, so it is crucial that less promising compounds are rejected early in the discovery phase before progressing to more expensive phases. This scenario impels researchers to refine and speed up the drug discovery process and to seek tools to support decisions related to modifications of the drug chemical structure to improve drugs' properties and thus increase the probability of success in the process of drug discovery. [1], [2] In the drug discovery process it should be considered that in physiological environment there will be reciprocal interactions between drugs and biological interfaces, such as cell membranes or plasma proteins, and from those interactions different pharmacokinetic profiles can be achieved. [3] Thus, it is important to develop i*n vitro* high throughput methods to evaluate the pharmaceutical profile, consisting in measuring properties such as permeability, lipophilicity, plasma protein binding, and biophysical changes of the membranes, which in turn affect other properties, such as the bioavailability of a drug and its pharmacokinetic profile. [4] Herein, the characterization of a newly synthesized drug (MIT-3) will be based on the measurement of fundamental biophysical properties, which allow inferring about its ADMET profile (absorption, distribution, excretion and toxicity at the membrane level). For this purpose, lipid-based colloidal nanosystems of different compositions were prepared as membrane mimetic models and several biophysical techniques were applied: derivative spectroscopy; quenching of steady-state and time-resolved fluorescence; quenching of intrinsic fluorescence of human serum albumin; synchronous fluorescence; dynamic and electrophoretic light scattering, differential scanning calorimetry and small and wide angle x-ray diffraction. The application of these techniques allowed to predict that MIT-3 has an ubiquitous location at the membrane level, presenting good membrane permeability and a good distribution in the therapeutic target. However, it is also predicted bioaccumulation with distribution in non-therapeutic targets and under conditions of prolonged exposure the drug may cause membrane toxicity as concluded by the impairment of membrane biophysical properties. It is also possible to conclude that the biophysical techniques and the biomimetic models used, constitute a toolbox of strategies for the future evaluation of other drugs.

Acknowledgements

This work was supported by the Portuguese Foundation for Science and Technology (FCT) in the framework of the Strategic Funding UID/FIS/04650/2013. We also acknowledge PEst-C/QUI/UI0081/2013, NORTE-01-0145-FEDER-000028 and PTDC/DTP-FTO/2433/2014. F. Cagide and S. Benfeito are thankful for the pos-doctoral and doctoral grants (SFRH/BPD/74491/2010 and SFRH/BD/99189/2013 respectively). Marlene Lúcio acknowledges the exploratory project funded by FCT with the reference IF/00498/2012. Eduarda Fernandes acknowledges COMPETE 2020 "Programa Operacional Competitividade e internacionalização".

References

[1] Y. Henchoz, B. Bard, D. Guillarme, P. A. Carrupt, J. L. Veuthey and S. Martel, Anal. Bioanal. Chem., 394 (2009) 707–729.

[2] J. Lin, C. Diana, S. M. F. de Morais, J. J. Xu, R. J. Polzer and S. M. Winter, Curr. Top. Med. Chem., 3 (2003) 1125–1154.

[3] H. Ferreira, M. Lúcio, C. Siquet and S. Reis, Química, 99 (2005) 39–51.

[4] E. H. Kerns, J. Pharm. Sci., 90 (2001) 1838–1858.

Self-assembledmolecular nanoparticles as new delivery systems

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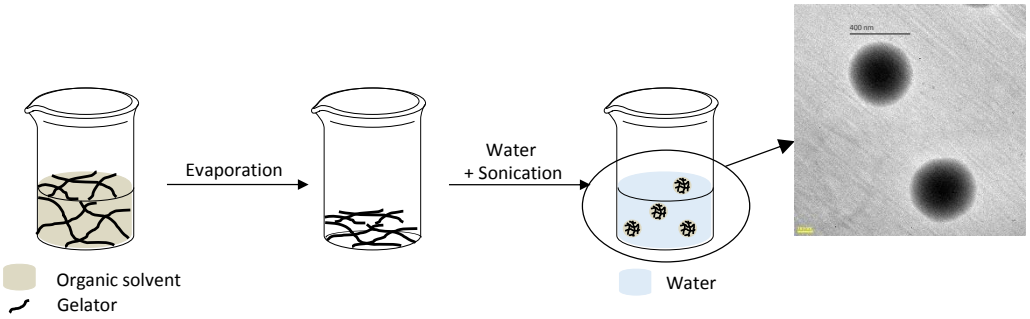
The need for nanocarriers arises from the increasing number of therapeutic and diagnostic agents whose efficacy is affected by nonspecific cell and tissue biodistribution, poor solubility or rapid metabolization and excretion. Miniaturization to nanoscale provides materials with a large surface area for bioconjugation, long circulation time in blood, and tunable size with the possibility of being actively or passively targeted to the desired site of action.

Among promising nanocarriers, nanogels have attracted much attention because, as hydrogels, they show high water content and biocompatibility. Other advantages are their simple preparation, high loading capacity, stability and responsiveness to environmental factors (such as ionic strength, pH and temperature). They have been reported to deliver their payload inside cells and to increase drug delivery across biological barriers [1].

Molecular gels, formed by the non-covalent association of low molecular weight molecules, have been extensively studied and present lots of potential applications (controlled release, tissue engineering, catalysis or optoelectronics) [2]. Although only polymeric nanogels have been studied so far, molecular gels characteristics make them appealing: they present a fully reversible and stimuli-regulated assembly and an easier biodegradation due to their small-molecule structure.

We present here the preparation and characterization of a new type of nanoparticles (ca. 100 nm) formed by self-assembled molecular gels. The approach used is the ultrasound-promoted nanogel formation, a fast and reproducible process [3]. The loading, stability and controlled release of different photoactive molecules has been studied, including in vitro experiments.



Acknowledgements
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References
[1] A. V. Kabanov and S. V. Vinogradov, Angew. Chem., 48 (2009) 5418-5429.
[2] R. G. Weiss, J. Am. Chem. Soc., 136 (2014) 7519-7530.
[3] X. Yan, Y. Cui, W. Qi, Y. Su, Y. Yang, Q. He and J. Li, Small, 4 (2008) 1687-1693.

TOPIC 2: SELF-ASSEMBLY

Ionic Surfactant-Carbon Nanotube Interactions. Use of Ion-Selective Electrodes

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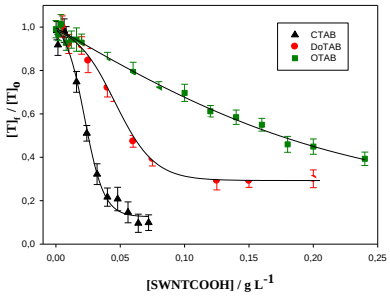
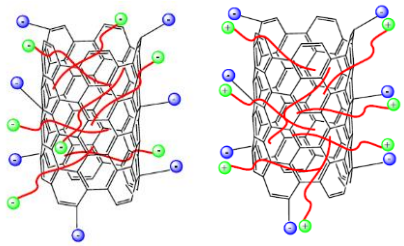
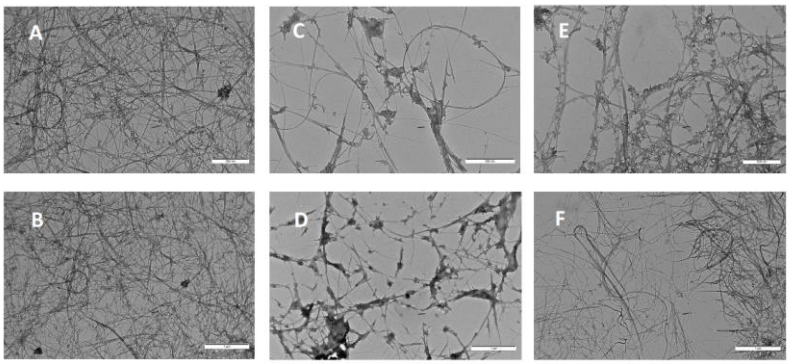
Carbon nanotubes, CNT, are building blocks used in the construction of molecular assemblies. Due to their mechanical, optical and electronic properties, they can be used in diverse fields. For instance, CNT have been used as sensors[1] or as vector in gene transfection[2]. The walls of the CNT are formed by curve sheets of graphene (or hexagonal laticce of carbon) which can provoke the assembly of the tubules into bundles due to attractive van der Walls and Π-stacking interactions. The separation (or dispersion) of such carbon nanotubules can be obtained by different methods. Surfactants are frequently used as dispersing agents.

The interaction of different cationic and anionic surfactants with functionalized and non-functionalized CNT has been studied in this work by using a potentiometric technique. Results show the cooperative character of the surfactant-CNT binding, as well as the importance of the hydrophobic interactions as driving force in such binding. A distinction in the use of the terms "dispersion" and "adsorption" has been established.







Acknowledgements
This work was supported by Consejería de Innovación, Ciencia y Empresa de la Junta de Andalucía (P12-FQM-1105), FQM-274 and FQM-206 and FEDER funds.

References
[1] J. Chen, T.O. Tran, M. T. Ray, D. B. Brunski, et al., Langmuir 29 (2013) 10586-10595.
[2] L. Shi, D. Shi, M. U. Nollert, D. E. Resasco, A. Striolo, J. Phys. Chem. B 117 (2013) 6749-6758.

Cationic colloidal system based on amino acid-based surfactants: characterization, antimicrobial properties and cytotoxicity

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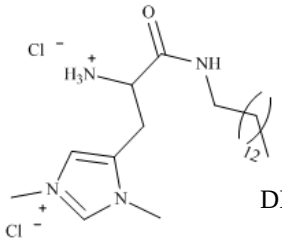
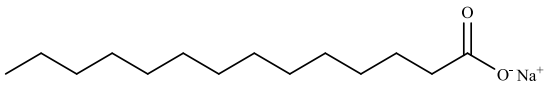
Nowadays, the design of efficient liposomal system for drug delivery is of considerable biomedical interest. Vesicles prepared from surfactant mixtures may offer several advantages due to their spontaneous formation and their long term stability [1]. However, despite the significant scientific interest and promising potential, the safety of vesicles systems remains a growing concern because of their unpredictable biological effects.

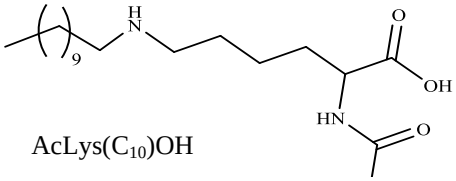
Recently our group has prepared monocatenary cationic histidine-based surfactants of different alkyl chain length. The polar head of these surfactants consists of the histidine amino-acid with methylene groups at N(π) and N(τ)-positions on the imidazole group of histidine. Given their simple chemical structure these new surfactants can be prepared using a straightforward and economical procedure. The C14 homologue ($DMHNHC_{14}$) showed remarkable growth inhibition activity against several Gram-positive and Gram-negative bacteria as well as fungi [2].



$DMHNHC_{14}$



$C_{13}COOH$



$AcLys(C_{10})OH$

Cationic colloidal systems composed by mixtures of the C_{14} homologue ($DMHNHC_{14}$) with sodium miristate ($C_{13}COOH$) or N-acetyl,N-Lauroyl lysine ($AcLys(C_{10})OH$) have been characterized by means of critical aggregation concentration, size distribution and zeta-potential measurements. The CAC values obtained for the $DMHNHC_{14}/C_{13}COOH$ and $DMHNHC_{14}/AcLys(C_{10})OH$ mixtures are much more lower than those showed by pure compounds. The structure of aggregates was studied using SAXS at Alba Synchrotron. The $DMHNHC_{14}/C_{13}COOH$ mixtures with high content of the histidine derivative contain vesicles with a mean diameter of about 250 nm and positive z-potential values. The $DMHNHC_{14}/AcLys(C_{10})OH$ mixtures shows viscosity and aggregates of different size (vesicles and micelles) has been observed by DLS. These formulations showed good stability and no separation phases were observed during six weeks.

The antimicrobial activity of these formulations decreases as the percentage of anionic surfactant increases. The cationic vesicles prepared with these mixtures show lower activity than that observed for the pure histidine surfactant. Cytotoxicity assays have been also performed using representative cell lines: 3T3· fibroblast, HaCaT keratinocytes and HeLa tumoral cell line.

Acknowledgements
We are grateful to I. Carrera for the technical assistance in the surface tension experiments. SAXS experiments were performed at the ALBA Synchrotron with the collaboration of ALBA staff. The beamtime at ALBA was kindly provided within the approved proposal n.2013110789.

References
[1] Pucci, C., Pérez, L., La Mesa, C. & Pons, R. Characterization and stability of catanionic vesicles formed by pseudo-tetraalkyl surfactant mixtures. *Soft Matter***10,** 9657–9667 (2014).
[2] M. Bustelo, A. Pinazo, M.A. Manresa, M. Mitjans, M.P. Vinardell, Pérez, Monocatenary histidine-based surfactants: Role of the alkyl chain length in antimicrobial activity and their selectivity over red blood cells, Colloids and Surfaces A, https://doi.org/10.1016/j.colsurfa.2017.04.017

Modulating supramolecular nanostructures: a free energy oriented approach

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Inclusion complexes have been used as building blocks for supramolecular structures such as polyrotaxanes, hydrogels and nanoparticles [1]. This often implies that the guest molecule is modified, so as to produce a dimer for connecting host-grafted chains, complementary host and guest-grafted chains, and other alterations to the basic structure. It is therefore useful to predict the effect that alterations in host and guest molecules produce for a known inclusion complex.[1,2] Focusing on the modification of the guest structure and the effect of non-included moieties in the binding constants (K_{bind}), an automated procedure based on molecular dynamics (MD) simulations and free-energy calculations with potential of mean force estimation was designed[1] for quantification of interaction and energy components, guiding complex formation in water between the model molecules. Different guest substituents including hydrophobic and hydrophilic moieties (with charged groups) are attached to a common backbone, the two naphthalene (NP) rings. Beta-cyclodextrin (CD) is used as a model host. Guest substituents clearly determine the overall inclusion behavior, allowing to double the free energy difference relative to the inclusion of the unsubstituted molecule, and increase the association constant more than 100-fold. Entropy does not favor inclusion and the order of magnitude of the binding free energy being given by the enthalpic component, with a dominating guest–host interaction contribution. Desolvation penalizes the inclusion process, and is not observed in the vicinity of the hydrophilic and charged groups, which typically are exposed to the solvent. For proper estimation of K_{bind}, substituent effects must be taken into account even if these substitutions do not appear to geometrically affect inclusion. This may also be relevant in supramolecular systems, in which a common guest group/moiety may coexist with different spacers or polymers. It is also seen that accurate predictions are available from MD, although further situations must be systematically assessed: the presence of substituents in the CD, and varying cavity volume. The prediction of favorable properties that govern the formation of host-guest complexes can be achieved imposing different substituents, paving the way for the modulation of relevant properties in supramolecular structures based on these complexes.

Acknowledgements
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References
[1] T.F.G.G. Cova, S.C.C. Nunes, A.A.C.C. Pais, *Phys. Chem. Chem. Phys*. 19 (2017) 5209-5221; [2]T.F.G.G. Cova, S.C.C. Nunes, T. M.V.D. Pinho e Melo, A.A.C.C. Pais.*Chem. Phys. Lett*. 672 (2017) 89-96.

Stoppering/unstoppering of a rotaxane formed between an N-heterocycle ligand containing surfactant:β-cyclodextrin pseudorotaxane and pentacyanoferrate(II) ions

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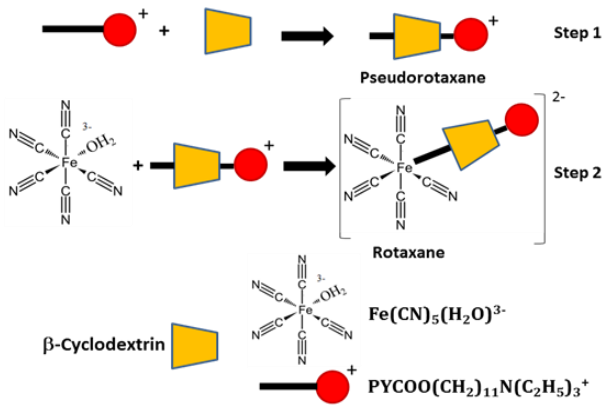
The potential applications of mechanically interlocked molecules, such as rotaxanes, have recently attracted much attention [1]. The studies on the formation of containing surfactants rotaxanes are scarce. In this work the preparation of a new kind of surfactant-based rotaxanes formed by a ligand substitution reaction between the aquopentacyanoferrate(II) ions and a suitable ligand located at the end of the hydrophobic tail of a surfactant threaded in a macrocycle, such as β-CD, was proposed. These rotaxanes can be unstoppered by a subsequent ligand substitution reaction with a higher field ligand than that present in the surfactant.

The surfactant11-(isonicotinoyloxy)-N,N,N-triethyl-1-undecanaminium bromide, 11PYBr,was synthesized and the formation of the pseudorotaxaneβ-CD:11PY$^+$, was studied by ^{1}H NMR and conductivity measurements (Step 1). Subsequently, the formation of the rotaxane by a ligand substitution reaction between the aquopentacyanoferrato(II) ions and the β-CD:11PY$^+$pseudorotaxane was investigated (Step 2). NMR spectra show that the rotaxane is formed through two different mechanisms.Kinetic data point out that the accessibility of the N donor atom of the pyridine to the five coordinated $Fe(CN)_5^{3-}$ intermediate is not much different in the absence and in the presence of β-CD.

In order to unstopper the rotaxane a strong or high-field ligand such as cyanide, CN^-, was added to the rotaxane solution. The unstoppering of the rotaxane was studied by ^{1}H NMR and kinetic experiments. However, there are other ways of unstoppering the rotaxane. DMSO could also be used as entering ligand instead of cyanide. On the other hand, it is also possible to use a redox reaction in order to unstopper the rotaxane.



The results of this work will provide a new general method to synthesize several new surfactant-based rotaxanes. The proposed method allows the preparation of many different rotaxanes by changing the nature of the ligand, the hydrophobic tail length, the number of hydrophobic surfactant chains, the charge of the surfactant and the nature of the macrocycle. Rotaxanes with intense solvatochromic behavior can also be prepared if azo-containing ligands are included, etc. That is, taking into account that changes in the hydrophilic and hydrophobic regions of surfactants can be relatively easy to achieve, the method described in this work will permit the preparation of several new rotaxanes. This is important since progress in the strategies to construct new supramolecular architectures broaden the scope of their use.

Acknowledgements
This work was supported by Consejería de Innovación, Ciencia y Empresa de la Junta de Andalucía (P12-FQM-1105), FQM-274 and FQM-206 and FEDER funds.

References
[1] Molecular catenanes, rotaxanes and knots: A journey through the world of molecular typology. J. P. Sauvage, C. Dietrich-Buchecker, Eds., Wiley-VCH, 2008.

Aggregation of cyclodextrins: insights into dynamic properties from NMR

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Cyclodextrins (CD) are a family of natural oligosaccharides formed by α-(1,4) linked glucopyranose units where the three first members are formed by 6, 7, or 8 glucopyranose units, denoted as α-, β-, or γ-cyclodextrin, respectively. Due to its toroidal structure CDs are able to form inclusion and non-inclusion complexes by interacting with a large variety of compounds, including inorganic, surfactants and non-polar drugs [1,2]. However, some of these processes are, according to several authors, affected by the presence of cyclodextrin aggregates. More than three decades ago, Miyajima et al. [3], based on viscosity and activity coefficients, suggested the formation of dimers, or larger aggregates, in aqueous solutions of α- and γ-cyclodextrin. One decade ago, Bonini et al. [4], based on static light scattering, DLS, and cryo-TEM, reported the formation of CD aggregates with a minimum hydration radius of ca. 90 nm. Subsequently, several researchers have discussed the formation of CD aggregates in aqueous solution [5].

Here we will discuss the aggregation of cyclodextrins on the basis of ^{1}H NMR self-diffusion and spin-relaxation rates (R_2) – the latter being a more sensitive parameter as it is related to the volume of particles [6]; following that, the behavior of deutered cyclodextrins will be analysed and discussed on the basis of the ^{2}H longitudinal relaxation times and its corresponding relaxation rates (R_1). The NMR analysis presented suggests that no larger aggregates are formed by CD, but the presence of aggregates with modest aggregation numbers cannot be ruled out.

Acknowledgements
This work was partially supported by the Fundação para a Ciência e aTecnologia (FCT), Portuguese Agency for Scientific Research,through the programmes UID/QUI/UI0313/2013 and COMPETE.

References
[1] T. Loftsson, M.E. Brewster, J. Pharm. Sci.85 (1996) 1017–1025.
[2] A.J.M. Valente, O. Söderman, Adv. Colloid Interface Sci.205 (2014) 156–176.
[3] K. Miyajima, M. Saweda, M. Nagakari, Bull. Chem. Soc. Japan56 (1983) 3556–3560
[4] M Bonini, S. Rossi, G. Karlsson, M. Almgren, P. Lo Nostro, P. Baglioni, Langmuir22 (2006) 1478–1484.
[5] T.T Do, R.V. Hooghten, G. V. Mooter, Int. J. Pharm., 521 (2017) 318-326.
[6] A.J.M. Valente, R.A. Carvalho, O. Söderman, Langmuir, 31 (2015) 6314–6320.

Molecular self-assembly of thiacyanine dyes into liquid crystals and silicatropic materials

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Cyanine dyes consist of two heterocyclic units, which are linked by an odd number of methine groups. They have applications in labeling, imaging, photopolymerization, and sensitized solar cells, among others [1,2]. Wepresent results on the self-assembly in water of a series of cationic thiacyanine dyes with variable molecular architecture, i.e. variable polymethine chain length and alkyl lateral substituents. UV-vis and fluorescence spectroscopy, and Nuclear Magnetic Resonance (NMR) analysis give evidence of dye face-to-face aggregation; which induces changes in optical absorption and fluorescence quenching. At higher dye concentrations we observed the formation of lyotropic (chromonic) liquid crystals providing the dye solubility is high enough; accordingly, too short or too long methine chains, or too long alkyl lateral substituents prevent mesomorphism. Liquid crystals change from nematic to hexagonal with increasing concentration; it was found that liquid crystals are formed by stacks with multimolecular cross section, similar to discotics. The studied cationic cyanine dyes can self-assemble cooperatively with silica species in a sol-gel reaction at alkaline conditions and produce silica nanofibers with dye stripes or mesopores (if the dye is removed) arranged hexagonally and oriented along the fiber´s long axis. These results demonstrate a facile strategy to obtain nanostructured fibers [3,4].

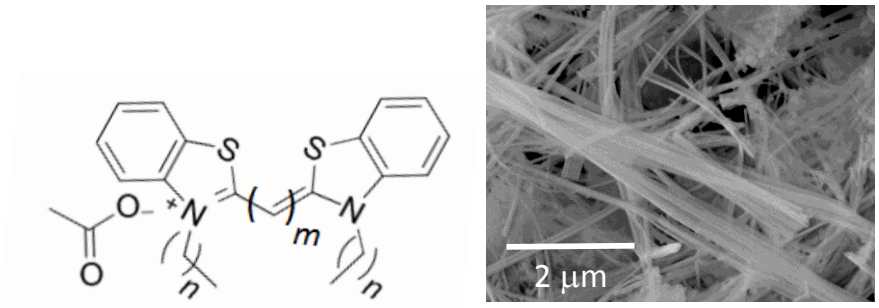

Figure 1: Chemical structure of studied thiacyanine dyes and example of derived silicatropic material

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References
[1] A. Mishra, R.K. Behera, P.K. Behera, B.K. Mishra and G.B. Behera, Chem.Rev., 100 (2000) 1973-2011.
[2] M. Henary and A. Levitz, Dyes Pigm., 99 (2013) 1107-1116.
[3] C. Rodriguez-Abreu, C. Aubery-Torres and G.J.T Tiddy, Langmuir, 27 (2011) 3067-3073
[4]C. Rodriguez-Abreu, C. Aubery-Torres, C. Solans, A. López-Quintela and G.J.T Tiddy, ACS Appl. Mater. Interfaces, 3 (2011) 4133-4

Tubular Nanostructures and Protein Binding in Lysine-based Surfactants

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Controlled and targeted drug delivery systems significantly improve the efficiency of drug delivery on the target cell, thereby minimizing the associated side effects. The development of intelligent vectors for controlled delivery of drugs is a stimulating scientific challenge with direct repercussions in the treatment of patients and high value of knowledge transfer. Amino acid-based surfactants are particularly promising systems [1], because of their high biodegradability and reduced human cytotoxicity. In addition to forming micelles and liposomes, they can self-organize into other complex supramolecular structures, such as fibers, twisted ribbons, helical tapes and nanotubes [2,3]. In this work, we have extensively characterized a family of anionic double-chained lysine-based surfactants, with variable degree of chain length mismatch, comprising compounds 8Lys*n* and *m*Lys8, and 10Lys*n* and *m*Lys10, with *n*, *m* = 12, 14 and 16; and the compounds 12Lys16/16Lys12, where the numbers represent the number of C atoms in each alkyl chain. To obtain further structural insight and investigate the mechanism of the different nanostructure formation, microscopic techniques such as video-enhanced light microscopy (VELM), scanning electron microscopy (SEM), cryogenic scanning electron microscopy (cryo-SEM), cryogenic transmission electron microscopy (cryo-TEM) and atomic force microscopy (AFM) were used (see figure). Since our subsequent aim is to employ the tubular aggregates as vehicles for biomolecules, a morphological and dynamic characterization by calorimetry of selected systems was performed, as a function of temperature and pH (stimuli associated with biomolecule release). Lastly, their interaction with different proteins, under varying experimental conditions, was further investigated, with the main goal of characterizing the fine structure of the m(Lys)n/protein aggregates formed.

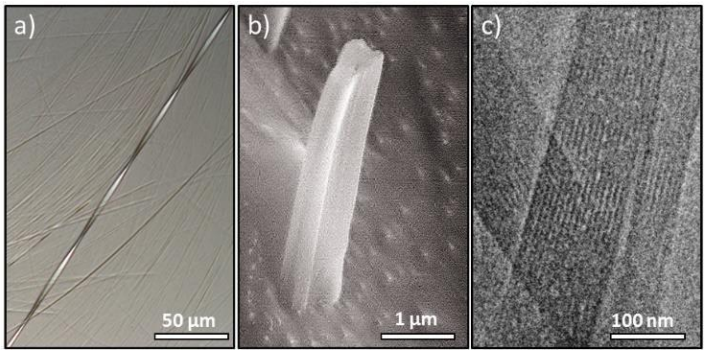

Figure. Tubular nanostructures of 8Lys16 in water (0.5% w/w) as observed by: a) VELM, b) cryo-SEM, c) cryo-TEM.

Acknowledgements
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References
[1] S.G. Silva, I.S. Oliveira, M.L.C. do Vale and E.F. Marques, Soft Matter, 10 (2014) 9352.
[2] T. Shimizu, M. Masuda, H. Minamikawa, Chem. Rev., 105 (2005) 1401.
[3] R.O. Brito, I.S. Oliveira, M.J. Araújo and E.F. Marques, J. Phys. Chem. B, 117 (2013) 9400.

Self-Assembly of Gold Nanoparticles based on Supramolecular Concepts

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In this communication, recent results regarding the development of aggregates of gold nanoparticles (AuNPs) with new type of colloidal morphologies will be presented.[1-4] We will show herein that the strategy of AuNPs self-assembly can be controlled by using supramolecular interactions in solution (Figure 1). The use of thiol-functionalized supramolecules to stabilize the surface of AuNPs can induce the spontaneous formation of supramolecular complexes or polymers,[1,2] which provides large and homogenous close packing of AuNPs, both in solution and interfaces. Once formed, the self-assembled superstructures have shown excellent levels of reversibility. The pH-, temperature- and pressure-controlled self-assembly may offer excellent reusable nanostructured materials to prepare functional materials in chiroptical sensing, photothermal therapy and molecular delivery.[3,4]

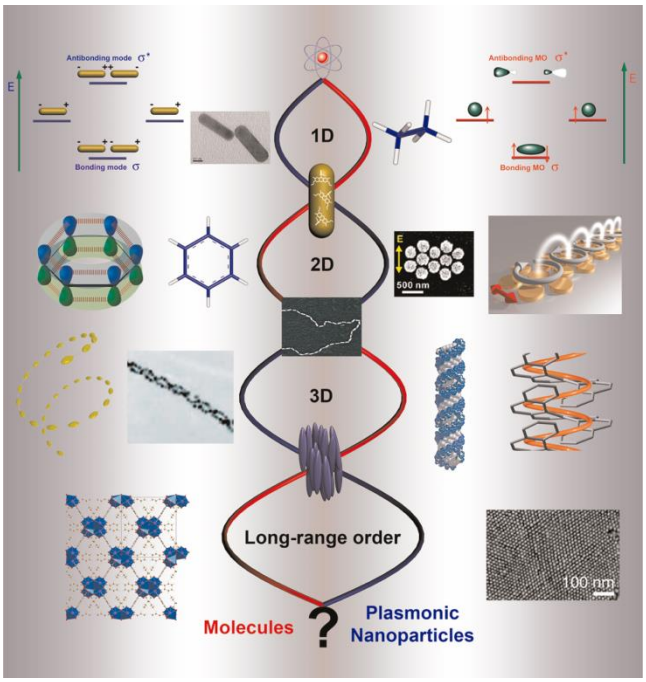

Figure 1. Nanoplasmonics based on supramolecular concepts.

References

[1] J. P. Coelho, G. González-Rubio, A. Delices, J. Osío Barcina, C. Salgado, D. Ávila, O. Peña-Rodríguez, G. Tardajos, A. Guerrero-Martínez. Angew. Chem. Int. Ed., 53 (2014)12751-12755.

[2] J. P. Coelho, G. Tardajos, V. Stepanenko, A. Rödle, G. Fernández, A. Guerrero-Martínez. ACS Nano, 9 (2015) 11241-11248.

[3] J. P. Coelho, M. J. Mayoral, L. Camacho, M. T. Martín-Romero, G. Tardajos, I. López-Montero, E. Sanz, D. Ávila-Brande, J. J. Giner-Casares, G. Fernández, A. Guerrero-Martínez. J. Am. Chem. Soc., 139 (2017) 1120-1128.

[4] R. Ahijado-Guzmán, G. González-Rubio, J. G. Izquierdo, L. Bañares, I. López-Montero, A. Calzado-Martín, M. Calleja, G. Tardajos, A. Guerrero-Martínez. ACS Omega, 1 (2016) 388-395.

Large-Scale Plasmonic Pyramidal Supercrystals via Templated Self-Assembly of Monodisperse Gold Nanospheres

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The unique optical properties of plasmonic gold nanoparticles are of great interest for the fabrication of novel materials.[1] In particular, their self-assembly into three-dimensional supercrystals has been exploited for metamaterials and light harvesting.[2,3] However, their acquisition requires the use highly regular building blocks. We have devised a facile and up-scalable method for the synthesis of gold nanospheres of various sizes and qualitative smoothness.[4] Based on the seeded growth method, large quantities of rough nanoparticles with diameters ranging between 10 and 110 nm are produced. Subsequent oxidative etching of the nanoparticles surface allows efficient removal of the roughness. Rational functionalization of the obtained gold nanospheres with thiolated polyethylene glycol and low surfactant concentration were found to produce optimal self-assembling behavior. By means of evaporative self –assembly combined with confined spaces as templates we produced uniform arrays of micron-sized 3D pyramidal supercrystals over large areas.

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References
[1] V. Myroshnychenko, J. Rodríguez-Fernández, I. Pastoriza-Santos, A. M. Funston, C. Novo, P. Mulvaney, L. M. Liz-Marzán, F. J. García de Abajo, Chem. Soc. Rev. 37 (2008) 1792-1805.
[2] Q. Liu, Y. Cui, D. Gardner, X. Li, S. He, I. I. Smalyukh, Nano Lett., 10, (2010), 1347-1353.
[3] C. Sartorio, S. Scaramuzza, S. Cataldo, V. Vetri, M. Scopelliti, M. Leone, V. Amendola, B. Pignataro, J. Phys. Chem. C,120, (2016), 26588-26599.
[4] C. Hanske, G. González-Rubio, C. Hamon, P. Formentín, E. Modin, A. Chuvilin, A. Guerrero-Martínez, L. F. Marsal, L. M. Liz-Marzán, J. Phys. Chem. C (2017), acs. jpcc.6b12161.

Magnetic Microdockers

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We will show different methods that allow for transporting micro-objects in a viscous fluid. At this scale the inertial forces are negligible as compared to the viscous ones and Navier-Stokes equations become time-reversible. As a consequence, the mechanisms of motion have to include some kind of flexibility or asymmetry.We will present different magnetic microdockers, made up of para- or ferromagnetic particles, that break the spatial symmetry thanks to the proximity of a boundary. The motion of these self-assembled microscopic structures results from the cooperative flow generated by their spinning components, which are also used topropel the colloidal species around, in a similar way to a hydrodynamic "conveyor-belt" [1,2].These systems adopt different geometries -chains, ring or squares- able to load and carefully transport inorganic cargos or biological cells, which is crucial in a large number of applications in microfluidics and biomedicine [3-5].

Acknowledgements
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References
[1] Martinez-Pedrero F., Ortiz-Ambriz A., Pagonabarraga I., and Tierno P. Phys. Rev. Lett. 115, 138301, 2015.
[2] Martinez-Pedrero F. and Tierno P. Phys. Rev. Applied 3, (2015) 051003,.
[3] Martinez-Pedrero F., Cebers A., and Tierno P. Phys. Rev. Applied 6, (2016) 034002.
[4] Martinez-Pedrero F., Cebers A., and Tierno P. Soft Matter 12, (2016) 3688.
[5] Martinez-Pedrero, F., Massana, H., Tierno, P., Small, (2017) 1603449.

Self-Assembly of Poly(N-Isopropylacrylamide-Methacrylic Acid) Microgels In Water

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A microgel composed by N-isopropylacrylamide and methacrylic acid (8mol%) [1] in water dispersions of 44 to 88 mg/mL was found to self-assemble originating a Photonic Band Gap (PBG). Depending on the concentration of the dispersion, the microgel self-assembles into a crystal or a glass phase with an elastic-solid rheological behavior. The resulting 3D periodic variation of the refractive index produces a strong visible light diffraction that is not allowed to propagate through the crystal/glass phase due to the PBG. This gives rise to structural color in the dispersions, that was found to be more blue when the elastic component is larger.
By increasing the temperature above the LCST of the polymer (~32°C), a concentration-dependent transition to a liquid phase occurs, with loss of color. Confocal microscopy further support the presence of the PBG and allow the visualization of the microgel particles ordering.

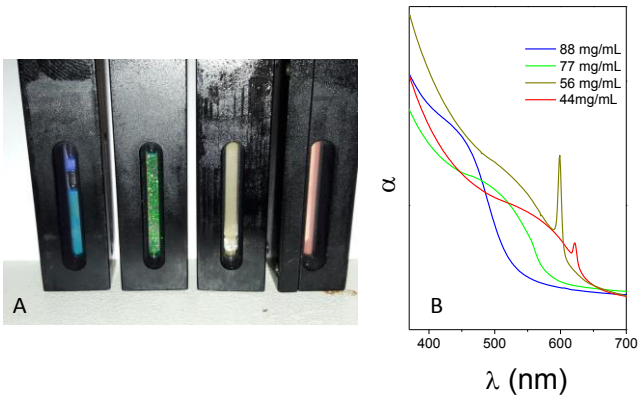

Fig.Microgel dispersions with decreasing concentrations from left to right (A) and variation of the turbidity (α) with wavelength (B).

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References
[1] Gema Marcelo, Laurinda R.P. Areias, María Teresa Viciosa, J.M.G. Martinho, José Paulo S. Farinha, *Polymer*116 (2017) 261-267. DOI: 10.1016/j.polymer.2017.03.071

Surface coverage and competitive binding of polymer and protein on carbon nanotubes

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Since carbon nanotubes are hydrophobic in character and thus do not disperse in water, covalent surface modification or addition of dispersing agents are usually needed [1,2]. Gauging the binding strength of dispersants, such as surfactants and polymers, onto the CNT surface is extremely valuable for optimizing dispersion efficiency or developing separation processes [1,2]. However, this problem is difficult to assess experimentally and thus data are scarce. Herein, we present results from self-diffusionNMR in dispersions of SWNTs prepared by either the block copolymer F127 or the protein bovine serum albumin, BSA [3,4]. The experiments detect the amount of F127 molecules adsorbed onto the SWNT surface. This quantity is recorded (i) in F127-SWNT dispersions to which BSA is added and (ii) in BSA-SWNT dispersions to which F127 is added. The data show that F127 molecules replace BSA ones adsorbed at the SWNT surface, while BSA leaves the adsorbed F127 coverage practically intact [4]. Consequently, F127 is found to bind more strongly to the nanotube surface than BSA. Hence, we provide an unambiguous method to evaluate dispersants by their adsorption strength.

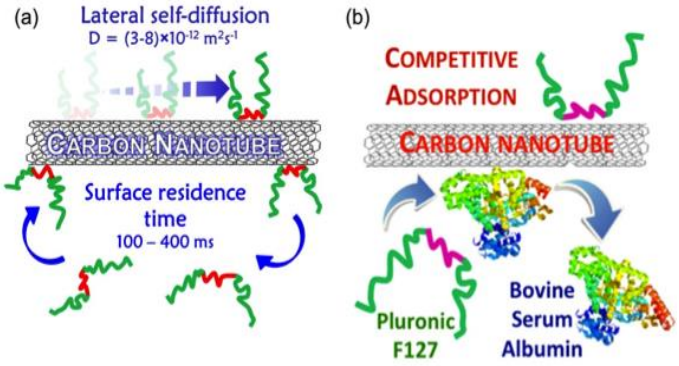

Figure 1. Main findings: (a) lateral diffusion of polymer along the nanotube and surface residence times; (b) competitive adsorption of polymer and protein onto the nanotube surface.

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References
[1] P. Angelikopoulos, H. Bock, Phys. Chem. Chem. Phys. 14 (2012) 9546.
[2] O.V. Kharissova, B.I. Kharisov, E.G. de Casas Ortiz, RSC Adv. 3 (2013) 24812.
[3] R.M.F. Fernandes, M. Buzaglo, M. Stein, I. Pri-Bar, O. Regev, E.F. Marques nd I. Furó, J. Phys. Chem. C 118 (2014) 582.
[4] R.M.F. Fernandes, M. Buzaglo, O. Regev, E.F. Marques, I. Furó, *J. Phys. Chem. C*, 119 (2015) 22

TOPIC 3: INTERFACES, MEMBRANES AND DISPERSED SYSTEMS

Surface Dilational Elasticity of Monolayers Adsorbed from Polyelectrolyte and Surfactant Mixtures

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Mixtures of polyelectrolytes and surfactants are attracting huge interests due to their ubiquitous nature. Polyelectrolytes are soluble in aqueous media, and mostly found in industrial and biological processes associated with neutral or charged surfactant. (1) These associations results in the formation of polyelectrolyte-surfactant complexes in the bulk liquid and at fluid-fluid interfaces. Polyelectrolyte-surfactant complexes adsorb at liquid-air interface to form thick layer which enhances the surface resistance to compression or shear and hence improves stability in systems such as foams. Dilational elasticity gives a measure of the surface resistance to compression or expansion. (2)
In this work, I have measured the surface dilational elasticity and viscosity of PDADMAC-SLES mixtures at the air-liquid interface in a wide frequency range (0.01Hz-1kHz). The low-frequency (0.01-0.1Hz) dilational properties were measured with the Oscillating Barriers technique (OB) while the Electrocapillary Wave Technique (ECW) was employed to measure the high-frequency properties (≥100Hz).

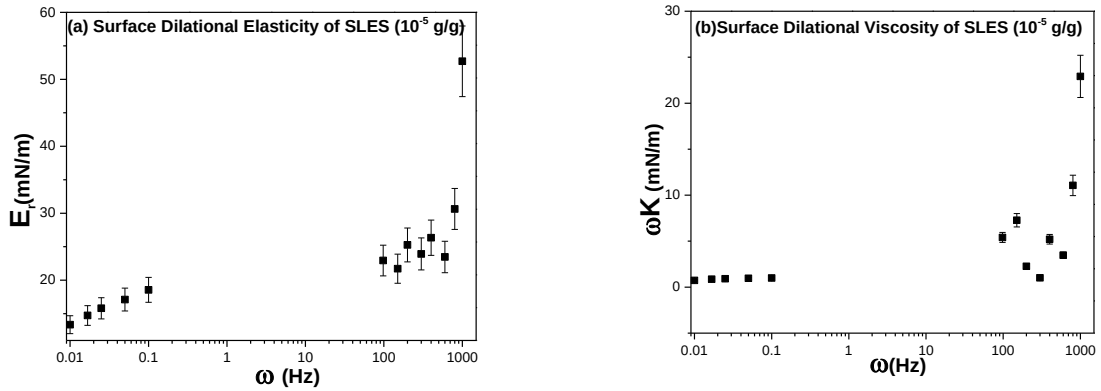

Fig: (a) Real and (b) Imaginary parts of Surface Dilational Elasticity as a function of frequency

The values of surface dilational elasticities observed were considerably high even at low frequencies as shown above.

References:

1) Bhattacharyya A., Monroy F., Langevin D., Argillier J-F. Surface Rheology and Foam Stability of Mixed Surfactant-Polyelectrolyte Solutions. Langmuir. 2000: 16: 8727-8732.
2) Goddard E.D., Grubber J.V. Principles of Science and Technology in Cosmetics and Personal Care. Cosmetic Science and Technology Series, vol. 22. Marcel Dekker; 1999.

Combining miniemulsion and solvothermal conditions for the synthesis of complex inorganic systems

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Nanodroplets of a liquid suspended in another immiscible liquid are able to confine spaces in which crystallization of both organic and inorganic materials can take place ("nanoreactors"), serving as "soft templates" for the formation of nanostructures [1]. The physical properties of liquids in nanodroplets can be substantially different from those of the bulk phase and the dynamics of the crystallization and melting processes are consequently affected. In particular, in so-called miniemulsions (a specific case of emulsions, kinetically stabilized by high-shear forces), the temperature of crystallization is significantly decreased with respect to the bulk phase because heterogeneous nucleation is practically suppressed.

So far, most of the investigations about the use of miniemulsions for confining crystallization processes have been carried out under mild conditions (low temperatures and ambient pressure) and,in general, for relatively simple compounds, mostly metal oxides. With this respect, in previous work we have reported the successful synthesis in inverse miniemulsion of different solid and hollow oxide nanoparticles, including CuO [2], Ce_2O, and γ-Fe_2O_3 [3] as representative examples. More recently, we have also extended the experiments to more complex ternary $Ce_{1-x}Cu_xO_2$ systems [4].

Here, we will reportour current work combining the miniemulsion technique with the nonstandard conditions provided by solvothermal routes, aiming to investigate the effects of increased pressure on the crystallization and on the properties of the resulting materials. The synergic combination of the two routes has allowed us to achieve transition metal spinel ferrites in highly crystalline form at lower temperatures (i.e., 80 °C) than usually required and without any post-synthesis thermal treatment [5]. This is an unprecedented result, affording a greener route to low temperature crystallization and avoiding the coalescence with the confinement provided by the droplets. We will also present our most recent investigations on the confined synthesis of ammonium phosphomolybdate nanoparticles and their application in catalysis.

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References
[1] R. Muñoz-Espí,Y. Mastai, S. Gross, K. Landfester,*CrystEngComm***2013**, *15*, 2175–2191.
[2] I. Singh, K. Landfester, A. Chandra, R. Muñoz-Espí, *Nanoscale***2015**, 7, 19250–19258.
[3] H. S. Varol, P. Dolcet, B. Kuerbanjiang, S. Gross, K. Landfester, R. Muñoz-Espí, *Langmuir***2016**, *32*, 13116–13123
[4] I. Singh, K. Landfester, R. Muñoz-Espí, A. Chandra, *Nanotechnology***2017**, *28*, 075601 (12 pp.)
[5] A. Antonello, G. Jakob, P. Dolcet, R. Momper, M. Kokkinopoulou, K. Landfester, R. Muñoz-Espí, S. Gross, *Chem. Mater*. **2017**, *29*, 985−997

Molecular Trends in Surfactant-Assisted Dispersions of Carbon Nanotubes

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The high aspect ratio and strong van der Waals cohesive forces (~40 kT·nm^{-1}) of carbon nanotubes (CNTs) results in tightly agglomerated, bundled powders. Surfactants have been used as non-covalent exfoliants and dispersants of pristine CNTs in water, but a fundamental understanding of the dispersing mechanism is still lacking [1]. Well-controlled, systematic dispersing methods and reliable comparative metrics are warranted. This could greatly influence optimization of dispersions and future applications. Herein, we have investigated the ability of several ionic surfactants to exfoliate and disperse single and multiwalled CNTs, resorting to a stringently controlled sonication-centrifugation method. In order to quantify CNT concentration, combined TGA and UV−vis spectroscopy were used. Different single-tailed and double-tailed gemini surfactants, covering a wide range of molecular properties, were studied [2-4]. The dispersibility curves obtained permitted the definition and comparison of several metrics. In turn, this allowed us to assess and rationalize the effect of different molecular properties (aromatic rings, chain length, headgroup charge, *cmc*, covalent spacer length) on the dispersing performance (*viz.* effectiveness and efficiency) of the surfactant.

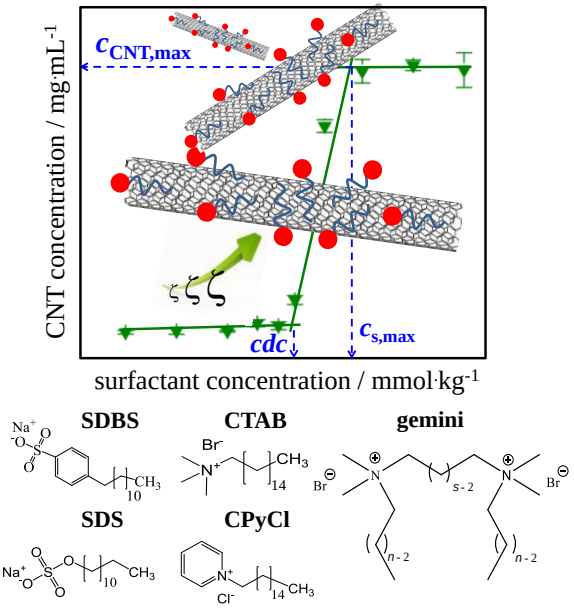

Figure 1. Performance metrics obtained from the dispersion curves for the different surfactants.

Acknowledgements

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References

[1] P. Angelikopoulos, H. Bock, Phys. Chem. Chem. Phys., 14 (2012) 9546-9557.

[2] R.M.F. Fernandes, B. Abreu, B. Claro, M. Buzaglo, O. Regev, I. Furó and E.F. Marques, Langmuir, 31 (2015) 10955-10965.

[3] R.M.F. Fernandes, M. Buzaglo, O. Regev, E.F. Marques, I. Furó, J. Phys. Chem. C, 119 (2015) 22190-22197.

[4] R.M.F. Fernandes, M. Buzaglo, O. Regev, I. Furó, E.F. Marques, J. Colloid Interface Sci., 493 (2017) 398-404.

Modelisation of the evaporation of a complex sessile droplet

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The evaporation of drop on surfaces is present in a lot of industrial and medical applications like printed electronics, spraying of pesticides, spray cooling, DNA mapping. Despite this strong interest, the dynamic of evaporation of complex liquid remains not fully understood.

The lifetime of a sessile droplet occurs in several steps. It starts with a stage of spreading followed by three different stages of evaporation. A first stage, where the contact line remains constant with a contact angle that decreases from an advancing to a receding contact angle.Then a second stage of evaporation where the contact line reduces with constant contact angle and finally a third stage where these parameters decrease simultaneously until the droplet completely disappears.

The effect of the composition on the evaporation of a sessile droplet is studied in the ambient conditions of temperature and relative humidity with various binary mixtures. A droplet of complex liquid is deposited on a substrate and the evolution of contact line and contact angle are simultaneously determined thanks to a droplet shape analyzer.

The values of the advancing and receding contact angles on PTFE substrate are estimated. Also, the experimental results for pure liquids are compared with a theoretical model developed by S. Semenov et al. [1] and a new model was developed to describe the binary case and shows good agreement for the 1st stage of evaporation.

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References
[1] S. Semenov, V.M Starov, R.G Rubio, H.Agogo, M.G. Velarde, Colloids and Surfaces A: Physicochem. Eng. Aspects (2011) 135-144.

Dissolution state of cellulose in aqueous systems.

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Cellulose is insoluble in water but can be dissolved in strong acidic or alkaline conditions. How well dissolved cellulose is in solution and how it organizes are key questions often neglected in literature but also a critical stepforward in the development of new efficient solventsystems for cellulose. Nevertheless, obtaining suchinformation is not trivial. The typical low or high pHs required for dissolving cellulose in acidic or alkaline solvents limits the use of typical characterization techniques. In this respect, Polarization Transfer Solid State NMR (PT ssNMR) emerges as a reliable alternative[1].
In this work, combining PT ssNMR, microscopic techniques and X-ray diffraction, a set of different acidic systems (phosphoric acid/water, sulfuric acid/glycerol and zinc chloride/water) and alkaline aqueous systems (NaOH, NaOH/thiourea and TBAH) are investigated[2, 3]. The studied solvent systems are capable to efficiently dissolve cellulose, although degradation occurs to some extent in acidic systems. PT ssNMR is capable to identify the liquid and solid fractions of cellulose, the degradation products and it is also sensitive to gelation. The regenerated materials were found to be highly sensitive to the solvent system used; typically less crystalline materials,presenting smoother morphologies, are obtained whenamphiphilic solvents or additives are used.

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References

1. Gustavsson, S., et al., *Polarization transfer solid-state NMR: a new method for studying cellulose dissolution.* RSC Advances, 2014. **4**(60): p. 31836-31839.
2. Alves, L., et al., *Dissolution state of cellulose in aqueous systems. 2. Acidic solvents.* Carbohydrate Polymers, 2016. **151**: p. 707-715.
3. Alves, L., et al., *Dissolution state of cellulose in aqueous systems. 1. Alkaline solvents.* Cellulose, 2015: p. 1-12.

Study of the adsorption of polyelectrolyte-surfactant mixtures at the water/vapor interface by neutron reflectivity and surface tension measurements

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The physico-chemical behavior of polymer – surfactant mixtures in bulk and upon adsorption at interfaces, both fluids and solids, attract big interest in recent years due to their recognized importance in many technological and industrial applications, ranging from drug delivery system to mineral processing, and from tertiary oil recovery to the development of cosmetic formulations for hair care.

In this communication, we study the adsorption at the water / vapor interface of mixtures composed by poly(diallyldimethyl)ammonium chloride, PDADMAC, and an anionic surfactant, sodium methyl-cocoyl-taurate (SCMT). For the purpose of this study, the pseudo-equilibrium surface tension isotherm has been analyzed using different tensiometers. In addition to the study of the pseudo-equilibrium isotherms, neutron reflectometry experiments have been carried out to draw a comprehensive scenario related to the adsorption of the complex mixtures. Surface tension and neutron reflectometry have provided information about the adsorption at the water / vapor interface of mixtures formed by (PDADMAC) and Sodium cocoyl methyltaurate (SCMT). Surface excesses obtained by neutron reflectivity show a monotonic increase with surfactant concentration, in agreement with the decrease of surface tension obtained using different tensiometers. However, interfacial tension measurements obtained for samples prepared using different mixing protocol evidences the existence of different aggregation patterns due to the formation of arrested aggregates, during solution preparation, that are not destroyed by dilution of the samples. Thus, the interfacial tension is dependent on the adsorption of the aforementioned aggregates at the water / vapor interface, leading to the appearance of surface tension peaks for polymer / surfactant ratio far from the two phase region. These results gather many possibilities for exploiting polymer – surfactant complexes in industrial applications such as cosmetic and drug delivery, due to the possibility to form quasi-solid-like aggregates for surfactant concentrations well below of the phase separation region.

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Phase transitions in fatty acids/alcohols Langmuir monolayers: Interfacial shear rheology results

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Insoluble surfactants on fluid-fluid interfaces form single molecule deep films that are called Langmuir monolayers. Such systems have been studied extensively on air-water interfaces because of their intrinsic interest as biological membrane model systems, their applications in many industrial processes, or as model systems to study the physics of two-dimensional systems.

Experiments on the thermodynamic properties and the microstructure of Langmuir monolayers have revealed an extraordinarily rich phase behavior. Particular emphasis has been made on fatty acid and fatty alcohol monolayers [1]. The mechanical properties of these systems have also been studied to some extent [2], but detailed knowledge about the rheological properties of the different thermodynamic phases appearing is still lacking. Technical limitations affecting both instrument resolution and long term measurement stability have precluded such studies.

The magnetic needle Interfacial Shear Rheometer [3] has recently been the object of interesting developments [4] that, by using magnetic tweezers to impose the probe motion, allow for a span of eight orders of magnitude in interfacial dynamic moduli. This is accomplished just by opting between two types of probe (a commercial one and a magnetic micro-wire [5]) and adjusting the magnification of the videomicroscopy system. Interfacial dynamic moduli as low as 10^{-9} N/m can be measured with this new type of interfacial rheometer. We will, first, describe the new rheometer design, its working principles and performance. Second, we will show that interfacial shear rheology is a useful tool in the study of phase transitions of fatty acids and alcohols Langmuir monolayers and we will report on a thorough study of the phase space of such monolayers through rheological measurements made with the new interfacial rheometer. Particular emphasis will be made in the study of the rheology of the untilted S and LS phases, where, by cross-checking the results of isothermal interfacial pressure sweeps and isobaric temperature sweeps, we will show a striking temperature dependence of the loss modulus of the viscosity dominated response in the LS phase that increases upon increasing the temperature [6].

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References
[1] V.M. Kaganer et al., Rev. Mod. Phys., 71 (1999) 779-819.
[2] C. Alonso et al., J. Phys. Chem. B, 110 (2006) 22185-22191.
[3] C.F. Brooks et al., Langmuir, 5 (1999) 2450-2459.
[4] J. Tajuelo et al., J. of Rheology, 60 (2016) 1095-1113.
[5] J. Tajuelo et al., Langmuir, 31 (2015) 1410-1420.
[6] L.E. Copeland et al., J. Chem. Phys., 10 (1942) 357-365.

Gemini Cationic Surfactants: Studying its Adsorption at Air/Water Interface and its micellization by ITC Calorimetry

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Gemini surfactants (dimeric surfactants) have increased its attention due to their high surface activity comparing that of the corresponding conventional (monomeric) surfactants. These surfactants appear to be better in certain properties than corresponding, and more conventional monomeric surfactants. Gemini surfactants are a group of surfactant molecules consisting of two hydrophobic tail and two hydrophilic headgroups connected through a spacer unit [1]. They are broadly classified into four categories depending on the types of headgroups (i.e. anionic, cationic, non-ionic and zwitterionic). Among them, cationic gemini surfactants are widely investigated categories because of their unique ability to form a complex with a variety of negatively charged molecules/particles and surfaces available in nature. Recently, in the field of surfactant science, the use of surfactants for the non-conventional application area has increased substantially. These areas of application include the use of surfactants as non-viral vectors for gene delivery, drug delivery agents, antimicrobial and antifungal agents, soft templates for the synthesis of mesoporous/microporous materials, and coating agents for nanoparticles/nanomaterials [2].

In this work, we have studied the surface activity at water/air interface and the micellization processes of three gemini cationic surfactants (α,ω-bis(S-alkyl dimethylammonium) alkane bromide). We focused on the equilibrium and kinetic behaviours of the cationic gemini surfactant at the air/water interface by using the pendant drop technique. Also we have investigated the effect of temperature on self-aggregation properties by isothermal titration calorimetry (ITC). Adsorption at air/water interface was modeled through analysis of the profile variation of a pendant drop, this profiles allow to calculate a dynamic surface tension using ADSA method. A model based at Frumkin adsorption isotherm and Ward-Tordai diffusion was developed to obtain characteristic parameters of the phenomena without using the Gibbs adsorption equation [3]. Different parameters like diffusion coefficient or maximum area per molecule were estimated by analysis of dynamic isotherms at different concentrations. Differences in same parameters between species was shown and interpreted. The isotherms of equilibrium surface tension values were used to estimate *cmc* values. The enthalpograms at different temperatures allow to study variations at *cmc* and energetic differences in dilution behaviour both monomer and micelle [4]. The results allow us to interpret the accommodation at interface and micellization of these surfactants.

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References
[1] R. Zana, Adv. Colloid Interface Sci, 97 (2002) 205-253.
[2] A. Bhadani, M. Tani, T. Endo, K. Sakai, M. Abe and H. Sakai, Phys. Chem. Chem. Phys., 17 (2015) 19474-19483.
[3] C.M. Phan, T.N. Le, C.V. Nguyen and S.-I. Yusa, Langmuir, 29 (2013) 4743-4749.
[4] H. Piekarski and K. Ludzik, J. Therm. Anal.Calorim. (2012) 110: 263-271

Emulsions containing essential oils: eco-friendly aqueous formulations of potential biopesticides for insect pest control

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Essential oils present a well-recognized bioactivity for insect pest control. However, their application is rather limited due to the difficulties associated with their distribution in the environment. Thus, the development of commercial formulations containing this type of components has been scarce in the last years. A promising alternative for their application is the development of new oil in water emulsion in which the essential oil can remain distributed as small droplets in a continuous phase formed by water. The main advantage of these formulations is that they are aqueous based formulations, thus making easy their application, and reducing their environmental impact.

We have studied three different types of formulations, containing essential oils, in which the stabilization of the emulsions is obtained by different phenomena. The first system is formed by free surfactant emulsion stabilized by the so called “pre-ouzo” (water/eugenol/ethanol system). A second type of system is formed by conventional emulsion stabilized by Pluronic F127, being the third system Pickering emulsions in which silica nanoparticles are added to the formulations containing Pluronic F127. One of the main characteristics of these emulsions is that they can be prepared by shaking midly the samples, leading to stable emulsions in a wide range of compositions.

As a proof of concepts, different insecticides (imidacloprid and azametiphos) were encapsulated inside the droplets, demostrating the applicability of the aforementioned formulations for pest control. Preliminary efficiency test of different formulations have shown better performance of these new formulations against different insects than conventional one. Thus, the results of this work open new perspective for designing new formulations with interest due to their enhanced bioactivity and biosustainability.

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Phospholipid/Nucleolipid Mixed Films for Guanine Recognition at the Air-Water Interface

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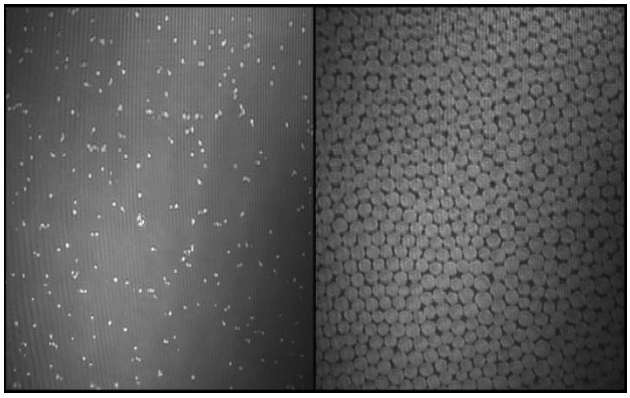
The Langmuir method offers the possibility of studying intermolecular interactions in thin films at the air–water interface with a high degree of detail. This work is framed in the development of a project aimed at describing the adsorption phenomenon of the DNA bases at a lipid matrix and the interactions by those complementary ones at the molecular level.

Nucleolipids are species formed by a lipid chain terminated in a nucleoside, capable of forming structures with high molecular recognition capabilities or "nucleolipoplexes"[1]. Nucleolipids are potential vectors for the distribution of drugs at the cellular level. Therefore, they have a great interest for their application in biomedicine.

In this work, we have studied the interaction of two DNA bases in environments that mimic the cellular interface. Langmuir monolayers of a pure nucleolipid 1,2-dipalmitoyl-sn-glycero-3-cytidine diphosphate (CDP-DG) have been fabricated at aqueous subphases. Also, thin mixed films containing 1,2-dipalmitoyl-sn-3-phosphate (DMPA)/CDP-DG were prepared. Such Langmuir films have been characterized by surface pressure–area isotherms, compression–expansion cycles and Brewster Angle microscopy (BAM)[2]. The influence of the pH, as well as the presence of the complementary Guanine base, has been investigated. These results combined with theoretical simulations led to propose a model of interactions between the nucleolipid and the complementary purine base.



Langmuir monolayer BAM images of CDP-DG in NaOH basic subphase (pH=11.5) (left) and in basic NaOH subphase (pH=11.5) with guanine 10^{-4} M (right). Both images have an anchor of 225 micrometers.

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References
[1] Milani, S.; Baldelli Bombelli, F.; Berti, D.; Baglioni, P. J. Am. Chem. Soc. 2007, 129, 11664–11665.
[2] Roldan-Carmona, C.; Giner-Casares, JJ.; Perez-Morales, M.; Martin-Romero, MT.; Camacho, L.; Adv. Coll. Int. Sci. 2012, 173, 12-22.

TOPIC 4: BIOCOLLOIDS

Bioreactors Engineered through Microfluidics

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Recent and parallel advances in the fields of membrane biophysics and genomics have enabled the reconstruction of minimal metabolisms within cell-like compartments. These compartments, droplets or vesicles, enable the isolation of genetic pathways from the external environment and thus may serve as efficient bioreactors [1]. Unfortunately, the lack of control of conventional production methods over the properties of the resultant droplets or vesicles holds further advance in the field, limiting the creation of artificial cells to simple proof-of-concept realizations. Further advance in the field requires a significant improvement over the encapsulation of genetic pathways within droplets or vesicles and their isolation from the environment by cell-like membranes. In this context, we propose to use microfluidic technologies to fabricate several hundreds of identical vesicles per second [2]. This technology enables us to encapsulate and isolate a DNA amplification system with a hundred percent encapsulation efficiency within a picolitter container, separating it from the environment by a cell-like lipid membrane. In particular, we encapsulate the phi 29 DNA Polymerase system [3], and quantify DNA amplification within these bioreactors by measuring the fluorescence intensity of Evagreen®, a fluorophore that emits only if bound to double-stranded DNA, within several cents of vesicles. Individual measurements on several hundreds of individual vesicles may help understanding the role of stochasticity during DNA amplification and therefore gene evolution.

Acknowledgements
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References
[1] Noireaux, V., & Libchaber, A. (2004). A vesicle bioreactor as a step toward an artificial cell assembly. Proceedings of the National Academy of Sciences, U.S.A. 101(51), 17669-17674.
[2] Arriaga, L. R., Datta, S. S., Kim, S. H., Amstad, E., Kodger, T. E., Monroy, F., & Weitz, D. A. (2014). Ultrathin shell double emulsion templated giant unilamellar lipid vesicles with controlled microdomain formation. Small, 10(5), 950-956.
[3] Blanco, L., Bernad, A., Lázaro, J. M., Martín, G., Garmendia, C., & Salas, M. (1989). Highly efficient DNA synthesis by the phage phi 29 DNA polymerase.Symmetrical mode of DNA replication. Journal of Biological Chemistry, 264(15), 8935-8940.

Layer-by-Layer Polyelectrolyte Microcapsules

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The layer-by-layer (LbL) self-assembly method has shown a wide range of applications in modern biotechnology,[1] e.g.. The LbL technique can be used for the fabrication of polyelectrolyte microcapsules for encapsulation and release of active compounds by the coating of colloidal templates such as micro- or nanoparticle, followed by the subsequent dissolution of this template[1]. These platforms present promising applications in drug delivery[2] and DNA encapsulation[3].

We present results relatedto the fabrication of polyelectrolyte microcapsules by the LbL coating of charged liposomes with layers of oppositely charged polyelectrolytes, thus it is possible to avoid the core dissolution step used when colloidal particlesare used as templates. In our work, we have used mixtures of the lipid dioleoylphosphatidylcholine (DOPC) and the charged surfactant dioctadecyl-dimethylammonium bromide (DODAB) to prepare liposomes of 50 nm radius by extrusion. The multilayers were built by the sequential adsorption of oppositely charged polyelectrolytes. We have used two different pairs, the first one formed bythe anionic poly(4-styrenesulfonate sodium salt) (PSS) and the cationic poly(allylaminehydrochloride) (PAH), presenting the second pair the same polyanion, PSS, and poly(diallyldimethylammonium) (PDADMAC) as cationic counterpart. These three polyelectrolytes present good properties to obtain physico-chemical insights on the process of the fabrication of the capsules. Furthermore, we have used two biocompatible polymers: poly-L-glutamic acid (PGA) and poly-L-lysine (PLL), negatively and positively charged, respectively and stable at physiological pH, in order to test the fabrication of biocompatible capsules with a more promising applicability. The characterization of the capsules formed was carried out by ζ-potential and dynamic light scattering measurements.

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References

[1] Decher, G.; Schlenoff, B., *Multilayer Thin Films: Sequential Assembly of Nanocomposite Materials*, ed Wiley-VCH, 2012
[2] Sukhorukov, G. B.; Rogach, A. L.; Garstka, M.; Springer, S.; Parak, W. J.; Muñoz-Javier, A.; Kreft, O.; Skirtach, A. G.; Susha, A. S.; Ramaye, Y.; Palankar, R.; Winterhalter, M., *Small***3**(6), 944-955, 2007
[3] Schukin, D. G.; Patel, A. A.; Sukhorukov, G. B.; Lvov, Y. M., *J. Am. Chem. Soc.*, **126**(11), 3374-3375, 2004

Hyaluronic Acid-Coated Liquid Lipid Nanocapsules as Delivery Systems Against Pancreatic Cancer Stem Cells

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Pancreatic cancer is currently the fourth cause of death related with cancer. The contributing factors for lethality include the lack of early symptoms, absence of accurate biomarkers for early diagnosis, rapid propensity for metastasis to the lymphatic system and distant organs, and the lack of effective chemotherapies. It has been recently established that these properties may be in part attributable to "cancer stem cells" (CSCs) [1], a small subpopulation of cells within tumors responsible for tumor initiation, growth, recurrence and chemotherapy resistance [2]. In this context, novel therapeutic strategies could be devised for targeting pancreatic CSCs, which would result in increasing drug sensitivity and causing inhibition of invasion and metastasis. For such purpose, liquid lipid nanocapsules (LLNs) constitute a new promising generation of drug-delivery systems due to their structure: an oily core able to include hydrophobic drugs and a surrounding protective shell which determines their capacity to survive in the circulatory system and also allows the inclusion of targeting molecules. Here, we have developed LLNs coated with different percentages of BSA and a targeting molecule for drug delivery on tumor cells, hyaluronic acid (HA). For further strengthen the protective protein layer, a cross-linking procedure with glutaraldehyde (GAD) was performed. Upon a dialysis cleaning process, BSA-HA coated LLNs showed improved colloidal stability respect to those only covered with BSA or HA. Cellular uptake assays were performed to assess the effectiveness of BSA-HA coated LLNs as a targeted drug delivery system against pancreatic cancer cells. Our final aim is to develop a suitable system for oral ingestion, so we also performed mucin interaction and digestibility assays. All the results obtained indicate that our BSA-HA coated LLNs represent a promising system for further investigations in the sphere of targeted drug delivery systems.

Acknowledgements
This work has been sponsored by the projects MAT2015-63644-C2-1-R and MAT2015-63644-C2-2-R.

References
[1] Rasheed ZA et al. *J Gastroenterol Hepatol*, 27(Suppl. 2), 2012, 15-18.
[2] Al-Hajj M et al. A *Proc Natl Acad Sci U.S.A*. 100, 2003, 3983–8.

May a Policationic Macrocycle Act as a Cationic Bridge Among an Anionic Lipid and a Plasmid DNA to Transfect Cells Efficiently?

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The use of cationic gemini lipids (GCLs) as safe nanocarriers of nucleic acids is one of the most promising approaches in the field of gene therapy (GT). However, some disadvantages, as their moderate toxicity and their interaction with serum proteins that favors phagocytosis, have promoted the study of other type of nonviral vectors. Among these, anionic lipids (ALs) have been found to be more biocompatible and less toxic than their cationic counterparts. But AL-DNA lipoplexes need the presence of a cationic entity that acts as an electrostatic bridge yielding an overall cationic complex able to overcome the electrostatic repulsion with the negative cell membrane. However, the transfection efficiency outcomes using divalent bridge cations as Ca^{2+}, Mg^{2+}, Mn^{2+} and Co^{2+} have proved to be less effective than those obtained with cationic lipids.[1] At this respect, a new approach to bridge AL-DNA interaction is proposed in this work, based on the use of a multivalent cationic macrocycle that yield a higher amount of positive charge per molecule than that obtained with divalent cations. The pillar[5]arenes are a new class of multivalent macrocyclic molecules composed of hydroquinone units linked by methylene bridges in their 2,5-positions, with ten positive charges (five charges at each end of the molecule).[2]In this work,[3] we have characterized the mixture formed by an anionic lipid (DOPG), the zwitterionic helper lipid (DOPE), a plasmid DNA and a pillar[5]arene macrocycle (P^{10+}). The idea is to check whether charge reversal is now reached and how this fact may improve transfection efficiency (TE). The study has been carried out using several biophysical experimental methods, such as, electrophoretic mobility/zeta potential, gel electrophoresis, small angle X-Ray scattering (SAXS), cryogenic electronic transmission microscopy (cryo-TEM), and atomic force microscopy (AFM), together with several biochemical experiments, such as gene transfection (FACS), cell viability/cytotoxicity, and protection against DNAses assays. The whole ensemble of biophysical and biochemical results of DOPG/DOPE-P^{10+}-pDNA lipoplex indicates that this system may open a novel and very promising via in the gene therapy field using anionic non-viral vectors mediated by multivalent cations.

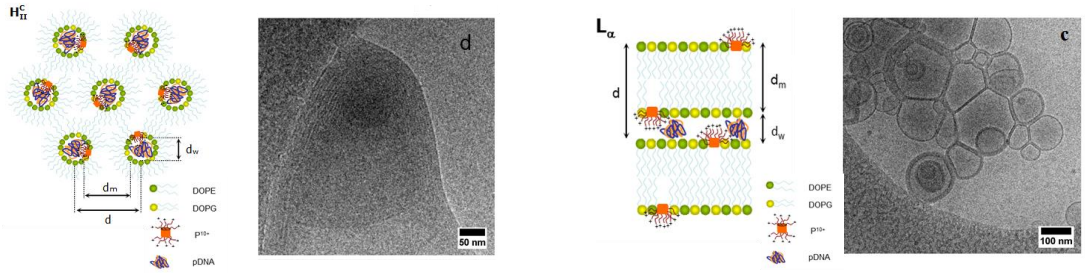

Figure 1. Schematical drawing of Hexagonal (H_{II}^C) and lamellar (L_a) phases of lyotropic liquid crystals found inDOPG/DOPE-$P10^+$-pDNA lipoplexes

References

(1) Srinivasan, C.; Burgess, D. J. *J. Controlled Release***2009**, *136*, 62.
(2) Ogoshi, T.; Kanai, S.; Fujinami, S.; Yamagishi, T. A.; Nakamoto, Y. *J. Am. Chem. Soc.***2008**, *130*, 5022.
(3) Barran-Berdon, A. L. M.-N., M.; García-Río, L; Domènech, O.; Tros de Ilarduya, C.; Aicart, E.; Junquera, E. *Journal of Materials Chemistry B***2017**, DOI: 10.1039/C6TB02939F. **HOT PAPER**

Colloidal characterization and in vitro study of olive oil immune-nanocapsules for directed drug delivery

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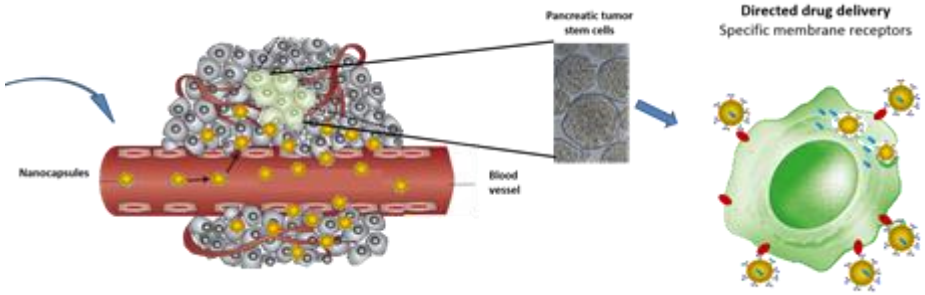
Lipid nanocapsules are promising nanocarriers for lipophilic drugdelivery. The surface characteristics of these colloidal particles are determinant in order to provide a controlled and directed delivery on target tissues with specific markers. We report the development of immuno-nanocapsules, in which a specific antibody (Anti-CD44) is conjugated to nanocapsules with the aim of a selective drug delivery to target cells. Specifically, this antibody interacts with the membrane receptor CD44 used as a cell-surface marker for several cancers [1]. A nanocapsule system was prepared by the solvent displacement technique obtaining an oily core surrounded by a functional shell with surface carboxylic groups [2]. A spacer molecule (polyethilene glycol, PEG) and the specific CD44 antibodies have been covalently conjugated with these nanoparticles through thesurface groups using a chemical method. A complete physico-chemical characterization of the immuno-nanocapsules was developed confirming the immobilization of PEG and antibody molecules on the colloidal nanoparticles. Finally, a preliminary "in vitro" study has been performed by culturing different (ealthy and tumoral) cell lines with nile-red loaded nanocapsules and immuno-nanocapsules with very promising results.



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References
[1] L.M. Negi, S. Talegaonkar, M. Jaggi, F.J. Ahmad, Z. Iqbal, R.K. Khar, Role of CD44 in tumour progression and strategies for targeting, J. Drug Target. 20 (2012) 561–573.
[2] P. Sánchez-Moreno, J.L. Ortega-Vinuesa, H. Boulaiz, J.A. Marchal, J.M. Peula-García, Synthesis and characterization of lipid immuno-nanocapsules for directed drug delivery: Selective antitumor activity against HER2 positive breast-cancer cells, Biomacromolecules. 14 (2013) 4248–42

Unravelling clathrin-mediated endocytosis

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Clathrin-mediated endocytosis is crucial for the internalization of most eukaryotic cell-surface proteins. Clathrin-coated vesicles (CCVs) assemble with their cargo at the plasma membrane then transport these to the early endosome inside the cell. A CCV consists of a clathrin scaffold coating a lipid vesicle, in which the cargo is embbeded, linked by adaptor proteins that are associated with effectors of CCV assembly, stability and disassembly.We recently determined that a single adaptor protein AP2 is sufficient to initiate and drive clathrin-coated bud formation on appropriate membranes, enriched in PtdIns(4,5)P2. [1,2]

In vivo, AP2 solely interacts with one leaflet of the cellular membrane. Therefore, an alternative approach is the direct measurement of clathrin assembly on a flat lipid surface (a Langmuir monolayer). By state-of-the-art soft matter characterization methods (including neutron scattering, interfacial tensiometry and rheology), we have been able to analyze the first stages of CCV assembly by using cargo embedded in a lipid monolayer.[3] We try to address here in particular the question of what influence does the AP2, and subsequently the clathrin scaffold have on the lipids.

References

[1] SE Miller, DJ Owen et al, *Cell.***147** (2011)1118-31.

[2] BT Kelly and DJ Owen, *Science.***345**, (2014), 459-63.

[3] A Maestro, N Zaccai, D Owen and P Cicuta, Submitted.

Effect of Cardiolipin on liposomes

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During cell division organisms like Escherichia coli regulate the distribution and composition of the lipids in their cell membranes. Cardiolipin is a negative curvature (cone shaped) phospholipid found on highly curvature places like poles and the region of the septum during cytokinesis. To study the effect of this lipid on the cell membrane and the possible interplay between molecular aspect and membrane curvature, we study the bending modulus of bilayer vesicles made of mixtures of DOPC and Cardiolipin. The experimental study is performed by exploiting the mechanical control of the thermal fluctuationsof giant unilamellar vesicles (GUVs) [1]. From the physical analysis we are able to measure the bending modulus of the liposomes as a function of the percentage of the Cardiolipin, which could unveils the mechanochemical role of this lipid during cell division.

Acknowledgements/Agradecimientos

References/Referencias

[1] Pécréaux J, Döbereiner HG, Prost J, Joanny JF, Bassereau P (2004) Refined contour analysis of giant unilamellar vesicles. Eur Phys J E 13: 277–290. doi:10.1140/epje/i2004-10001-9.

Polymeric particles and membranes for cell encapsulation, proliferation and release

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Polymeric nanoparticles, films and scaffolds are regarded as exceptional materials for diverse biomedical applications such as drug delivery, tissue engineering and repair, etc [1]. However, the synthesis of these particular materials os their surface modifications commonly involves the use of organic/toxic solvents and additives, sacrificial templates that have to be removed at post-production stages, sophisticated instruments and/or extreme working conditions of temperature and pressure, compromising both the integrity of diverse bioactive compounds and the process yield [2-3].
Filling this gap, we here describe biologically-friendly strategies to produce millimeter-size hollow polymeric particles and cross-linked polymeric membranes for potential applications in the biomedical field. In particular, hollow particles were produced from droplets of DNA and methacrylamide chitosan aqueous solutions(CH:MA), which were assembled and hardened by a double ionic/covalent superficial crosslinking on top of superhydrophobic surfaces, leading to liquid-core particles with a hardened hydrogel shell. The particles display softness to the touch and an outstanding structural stability against manipulation by hand and with forceps. Meanwhile, cell staining, fluorescence microscopy, and MTT proliferation assay revealed that the liquid DNA guaranteed a biocompatible médium for effcient cell encapsulation and survival followed by a superior release and proliferation of viable cells, as compared to solid CH:MA particles used as controls. On the otehr hand, polymeric membranes were obtained by solvent casting followed by a cross-linking step mediated by the chemical vapor deposition (CVD) of glutaraldehyde (GA). The membranes were characterized against non- and solution cross-linked membranes in terms of their mechanical/surface properties and biological performance. Among others, the CVD membranes proved (i) to be more mechanically stable against cell culture and sterilization than membranes cross-linked in solution and (ii) to prompt the adherence and sustained proliferation of healthy cells to levels even superior to commercial tissue culture plates (TCPs). Based on the obtained results, the produced hollow particles and polymeric membranes hold promise for tissue engineering and regenerative medicine, where manipulable and biocompatible synthetic carriers (implants) are often needed to supply living cells and other sensitive bioactive compounds. Moreover, the described strategies per se might be of interest to researchers working at the interface of polymer science, biology, and biomaterials inasmuch as it proves to be simple, reproducible, cost-effective, and totally biocompatible, not requiring the use of sophisticated experimental set-ups and/or potentially harmful procedures.

Acknowledgements
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References
[1] M. Sokolsky-Papkov, K. Agashi, A. Olay, K. Shakesheff, A. J. Domb, Adv. Drug Deiv. Rev., 59 (2007) 187-206
[2] T. Shao, X. Feng, Y. Jin, Y. Chen, Chem. Eng. Sci., 104 (2013) 55-63.
[3] Z. Liu, X. Xu, R. Tang, Adv. Funct. Mater., 26 (2016) 1862-1880.

Effect of NaCl on the aggregation behavior of rhamnolipids and implications in their biological activity

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Rhamnolipids are a class of glycolipid biosurfactants produced mainly by *Pseudomonas aeruginosa* strains. Their structure comprises one or two rhamnose molecules linked to one or two β-hydroxy fatty acids which can differ in the chain length and the degree of saturation. Rhamnolipids display a similar or better performance when compared with chemical surfactants, and exhibit higher biodegradability and lower toxicity, which make them potential alternatives to the synthetic surfactants in several applications [1]. Among them, rhamnolipids can be used as an alternative to the chemical fungicides to prevent the contamination and deterioration of agriculture products by fungi. In this work, the antifungal activity of rhamnolipids produced by *P. aeruginosa* #112 was evaluated against *Aspergillus niger*MUM 92.13 and *Aspergillus carbonarius*MUM 05.18. These species are among the most common fungal contaminants, and represent a health risk due to the production of mycotoxins. *P. aeruginosa* #112 produced eight different rhamnolipid congeners (including mono- and di-rhamnolipids). The growth inhibition percentages obtained for both fungi with the crude rhamnolipid mixture (3 g/L) were between 22 and 28%. Subsequently, it was studied the effect of different electrolytes in the antifungal activity of rhamnolipids. It was found that the growth of *A. carbonarius*MUM 05.18 and *A. niger*MUM 92.13 was completely inhibited by a combination of the crude rhamnolipid mixture (3 g/L) and NaCl (at concentrations between 375 and 875 mM). In order to establish a relationship between the antifungal activity and the aggregation behavior of rhamnolipids, the size distribution of the self-assembled structures formed by the crude rhamnolipid mixture in aqueous solution was studied at different NaCl concentrations through Dynamic Light Scattering. In the absence of NaCl, rhamnolipids formed micelles with an average size around 300 nm. The addition of NaCl resulted in an increase in the size of the structures formed, and for the highest NaCl concentration tested (875 mM), the average size of the self-assembled vesicles was higher than 2 μm. The formation of these large vesicles by rhamnolipids in the presence of NaCl was confirmed through Confocal Scanning Laser Microscopy. The results obtained demonstrated a relationship between the antifungal activity of rhamnolipids and their aggregation behavior, which opens the possibility to improve their biological activities for application in different fields.

Acknowledgements
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References
[1] E.J. Gudiña, A.I. Rodrigues, V. de Freitas, Z. Azevedo, J.A. Teixeira, L.R. Rodrigues, Valorization of agro-industrial wastes towards the production of rhamnolipids. Bioresource Technology. 212 (2016) 144-150.

Gold Nanorods in Surface-Enhanced Raman Spectroscopy as a Toxicological Tool for Cocaine Detection

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Cocaine (COC) is the second most consumed drug all over the world, after marijuana, with strong effects on human behaviour. The techniques employed up to date for this purpose are cost- and time-consuming, and generally require complex sample pretreatment.

Here, Raman spectroscopy has been investigated as an alternative methodology, in order to perform rapid and non-destructive analysis. This work describes the first application of surface-enhanced Raman spectroscopy (SERS) to the analysis of non-pretreated oral fluid samples doped with COC because, differently from the previously published papers [1-4], in this work neither extraction nor preconcentration were performed.

For SERS analyses, gold nanorods have been synthetized by a seed-mediated process, and then characterized by Ultraviolet spectroscopy, transmission electron microscopy and Raman spectroscopy. Since synthetized nanorods showed a very intense absorption band in the Infrared region, synthesis parameters were tuned in order to create a resonance with the infrared laser employed (780 nm).

As a result, a large improvement in the detection of COC in non-pretreated oral fluid samples was observed. The lowest limit of detection (LOD =10 ng/mL) obtained with spectroscopic techniques, among the ones published up to date, has been achieved. Besides, it has been demonstrated that, with this substrate, ultratraces of COC can be detected in oral fluid without the need of a sample pretreatment.

Acknowledgements
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References
[1] C. Shende, F. Inscore, P. Maksymiuk and S. Farquharson, Proc. SPIE-Int. Soc. Opt. Eng. 6007 (2005), 60070S/1-60070S/7.
[2] F. Inscore, C. Shende, A. Sengupta, H. Huang and S. Farquharson, Appl. Spectrosc., 65 (2011) 1004-1008.
[3] S. Farquharson, C. Shende, A. Sengupta, H. Huang and F. Inscore, Pharmaceutics 3 (2011) 425-439.
[4] JK. Dana, C. Shende, H. Huang, S. Farquharson, Anal. Bioanal. Tech. 6 (2015), 289-293.

TOPIC 5: POLYMERS AND GELS

Computer simulations of interaction forces between nanogels

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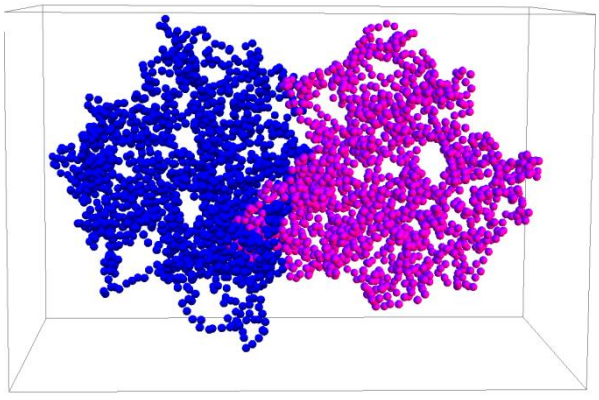
In the last decades, micro- and nanogels have attracted considerable attention due to their versatility and high sensitivity to external stimuli. In addition, these nanoparticles bridge the gap between classical hard colloids and ultra-soft polymeric colloids and are employed in experiments addressing condensed matter issues such as structure formation, dynamics or phase transitions.

The precise knowledge of the forces between nanogels is essential in any attempt to understand their behavior and control the processes in which they are involved. In spite of its relevance, there are relatively few papers dealing directly with the effective interactions between these nanoparticles. More specifically, there are just a few works on the forces between two nanogels when they come into contact, usually referred to as elastic or steric forces. The simple soft-sphere potential and the Hertzian potential are the two theoretical formalisms mostly employed until now by some authors to quantify interactions between nano- and microgels in contact. Accordingly, explicit coarse-grained Monte Carlo simulations have been performed to find out if these models can capture the interactions between overlapping neutral nanogels [1]. In the case of the Hertzian potential, this work also provides: i) a relationship between the effective (or nominal) diameter appearing in the expression for this potential and a geometrical diameter; ii) a procedure to obtain a first estimate of the other parameter characterizing this potential, its strength, from some theoretical expressions and coarse-grained simulations. The previous items can be appealing for many experimentalists and theorists since an approximate prediction of the elastic force can be made from them.



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References
[1] S. Ahualli, A. Martín-Molina, J.A. Maroto-Centeno and M. Quesada-Pérez, Macromolecules, 50 (2017) 2229−2238.

Microgels obtained in water-in-water (w/w) emulsions

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Water-in-water (W/W) emulsions are liquid/liquid dispersions of two immiscible aqueous phases, in absence of both oil and surfactant. These colloidal dispersions can be prepared in aqueous mixtures of two hydrophilic polymers, in which segregative phase separation occurs because of mutual incompatibility between the two polymers [1,2]. The present work focuses on the study of emulsion droplets in H_2O/protein/polysaccharide systems. Different methods of emulsion formation have been studied, and the results have demonstrated that small droplets can be obtained by fast nucleation, inducing a phase transition from a single-phase region to a two-phase region of the phase diagram.

Gelatin microgels have been obtained by gelification of the dispersed phase of W/W emulsions, by decreasing temperature in gelatin-rich droplets. The stability of such microgels has been greatly improved by crosslinking with genipin. The encapsulation of active components inside these microgel particles has also been studied.Fig. 1 shows an example of gelatin microgels, obtained by dispersing a gelatin aqueous solution into a maltodextrin aqueous solution at 50ºC, and then cooling down to 25ºC.

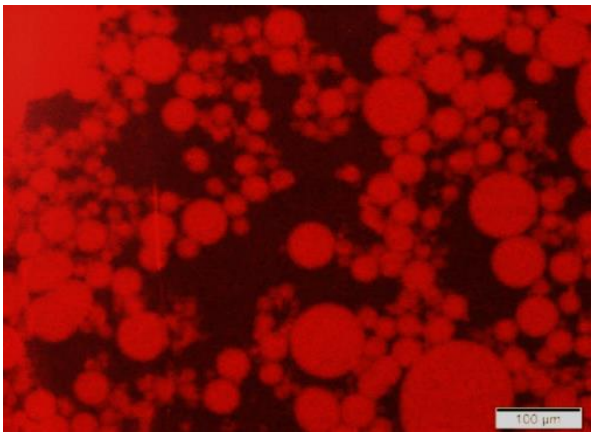

Fig. 1. Optical microscopy image of gelatin microgels, observed by fluorescence optical microcopy using gelatin labeled with rhodamine.

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References
[1] T. Nicolai, B. Murray, Particle stabilized water in water emulsions, Food Hydrocolloids, 2016
[2] J. Esquena, Water-in-water emulsions, Current Opinion in Colloid and Interface Science, 25 (2016) 109

Role of charge distribution in the absorption of biomolecules in ionic microgels

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Ionic microgels are charged colloidal particles of gel dispersed in a solvent, formed by cross-linked polyelectrolyte chains. They can swell or shrink in response to a wide variety of stimuli such as temperature, pH, salt concentration or solvent nature. This feature is an advantage for a wide number of biotechnological applications. In particular, the design of drug transport and delivery systems is gaining attention in recent years. With this aim, several studies have been developed to study the permeation of ions and solutes inside microgels particles [1-3]. In this work we have theoretically studied the uptake of a non-uniformly charged biomolecule, suitable to represent a globular protein or a drug, by a charged microgel in the presence of 1:1 electrolyte. Based on the analysis of a physical interaction Hamiltonian, we have identified five different sorption states of the system, from complete repulsion of the molecule to its full sorption deep inside the microgel, passing through meta- and stable surface adsorption states. The results are summarized in state diagrams that also explore the effects of varying the electrolyte concentration, the sign of the net electric charge of the biomolecule, and the role of including excluded-volume or hydrophobic biomolecule-microgel interactions. We show that the dipole moment of the biomolecule is a key parameter controlling the spatial distribution of the globules. In particular, biomolecules with a large dipole moment tend to be adsorbed at the external surface of the microgel, even if like-charged, whereas uniformly charged biomolecules tend to partition towards the internal core of an oppositely-charged microgel. Hydrophobic attraction shifts the states towards internal sorption of the biomolecule, whereas steric repulsion promotes surface adsorption for oppositely-charged biomolecules, or the total exclusion for likely-charged ones. Our results establish a guidance for the spatial partitioning of proteins and drugs in microgel carriers, tunable by microgel charge, pH and salt concentration.

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References
[1] A. Moncho-Jordá, I. Adroher-Benítez, *Soft Matter* 10 (2014) 5810-5823.
[2] I. Adroher-Benítez, S. Ahualli, A. Martín-Molina, M. Quesada-Pérez, A. Moncho-Jordá, *Macromolecules* 48 (2015) 4645–4656.
[3] I. Adroher-Benítez, S. Ahualli, D. Bastos-González, J. Ramos, J.Forcada, A. Moncho-Jordá, *J. Polym. Sci. Part B Polym. Phys.* 54 (2016) 2038-2049.
[4] I. Adroher-Benítez, A. Moncho-Jordá, and J. Dzubiella, *Langmuir* (under revision).

Soft self-assembled nanoparticles for gene and drug delivery

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Formulations based in lipid systems (e.g. liposomes) hold the promise of becoming safe and efficient delivery systems for drugs and genes in therapeutic applications [1,2]. Yet, the efficiency of such systems is still relatively low and further progress in the technology is needed to achieve the required performance for therapeutic applications.

In this presentation I will talk about our recent advances in the development of novel methodologies capable of making soft self-assembled nanoparticles of controlled size and nanostructure, and which are capable of incorporating polar and apolar drugs simultaneously.

References

[1] T. M. Allen, P.R. Cullis, Adv. Drug Deliv. Rev., 65 (2013) 36–48.
[2] B. F. B. Silva, R. M. Majzoub, C.-L. Chan, Y. Li, U. Olsson, C. R. Safinya, Biochim. Biophys. Acta-Biomembr., 1838 (2014) 398–412.

PNIPAM-Based Microgels with a UCST Response

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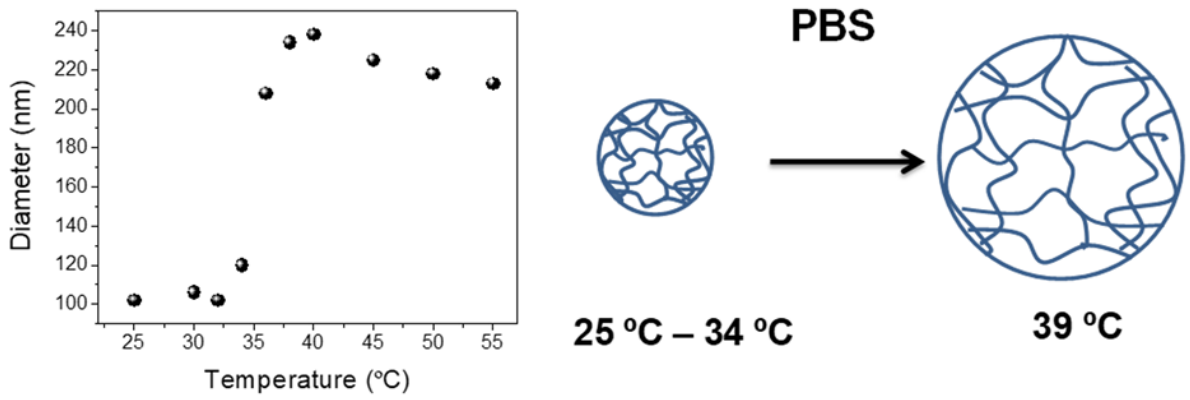
Microgels based in poly(N-isopropyl acrylamide), pNIPAm, are widely used due to their lower critical solution temperature (LCST) in water. [1] Here we present a novel pNIPAm-based copolymer gel with exactly the opposite behavior, i.e., presenting an upper critical solution temperature (UCST) in buffer solution. The gel nanoparticles contain 92mol% of pNIPAm, 2-(3,4-dihydroxy-6-nitrophenyl)ethyl methacrylamide (nitroDOMA), methacrylic acid (MAA),and methyl bis-acrylamide crosslinker (MBA),and show a surprising UCST transition in physiological conditions, with the diameter increasingmore than 150% from 34ºC to 40ºC. [2]

The unusual properties of this material are due to the small fraction of copolymerized MAA and nitroDOMA monomers. The collapsed conformation in PBS buffer below 34ºC is stabilized by hydrogen bonding, with repulsion from the partially ionized nitrocatechol and methacrylic units screened by the ionic strength and the formation of hydrophobic clusters by the methyl groups of MAA. The increase in temperature leads to the collapse of pNIPAm segments, which disrupts the balance of supramolecular interactions, leading to the large volume expansion of the gel. [2]



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References
[1] J.P. Pinheiro, L. Moura, R. Fokkink, J.P.S. Farinha, *Langmuir* 28 (2012) 5802-5809. DOI: 10.1021/la2045477
[2] Gema Marcelo, Laurinda R.P. Areias, María Teresa Viciosa, J.M.G. Martinho, José Paulo S. Farinha, *Polymer*116 (2017) 261-267. DOI: 10.1016/j.polymer.2017.03.071

POSTER SESSION

Release of acyclovir from polymeric nanofibers: comparingaqueous versus membrane-water interfaceskinetics

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Introduction: Acyclovir (ACV) is a guanosine antiviral prodrug most commonly used for the treatment of infections caused by: *Human alphaherpesvirus* (HSV) 1 and 2; *Human alphaherpesvirus* 3 (VZV) and *Human gammaherpesvirus* 4 (EBV) [1]. ACV is phosphorylated by thymidine kinases in infected host cells and converted to di- and triphosphates derivatives. These compounds are responsible for ACV inhibitory effects on DNA polymerase [2]. However, this antiviral drug has several limitations. According to the Biopharmaceutical Classification System, ACV can be classified as a class III or IV drug because of its low permeability and solubility. ACV has low bioavailability and the drug mean plasma half-life is about 2.5 hours, hence, repeated administration of high doses (200-800 mg, five times daily for 10 days) is needed for the treatment of HSV infections [3,4].

Objective: The objective of this study is to develop a novel system of controlled release of ACV for cutaneous application through the encapsulation of the drug into polymeric nanofibers produced by the electrospinning technique to overcome the limitations of the conventional topical formulations.

Method: The nanofibers composition and preparation method were optimized and the final nanofibers produced were characterized by Scanning Electron Microscopy with Energy-Dispersive X-ray Spectroscopy (SEM-EDS) for topographic and elemental analysis of the samples. X-ray diffraction was also used for the structural characterization. Controlled release assays were carried out at physiological conditions (pH 5.5 and 37 ºC) in aqueous or in micellar environment (to mimic the biological interface). Controlled release assays of the formulations developed were compared to the commercial topical formulation (Zovirax® cream). Cellular viability (MTT assay) was also assessed using HaCaT human epidermal keratinocytes and HFF-1 human foreskin fibroblasts.

Results: The nanofibers produced had an average cross-sectional diameter value of 595 nm. The diffractogram and SEM-EDS analysis revealed the presence of ACV in nanofibers. The controlled release assay performed in aqueous environment showed a total drug release of 7.3 ± 1.0 % against 98.1 ± 9.9 % release when performed in micellar environment. The same tests performed in the commercial formulation have shown percentages of drug release of 80.2 ± 2.0 % and 69.0 ± 1.7%, respectively. The release profile of ACV from the commercial formulation was however very different from the developed nanofibers, the later presenting a more sustained release during 199 hours against the more immediate release of commercial formulation in 52 hours. The nanofibers presented acceptable cellular toxicity up to a concentration of 25 mg/mL.

Conclusions: The electrospinning technique was efficient in producing ACV-loaded nanofibers, being a promising approach to reach a more sustained drug release profile. Moreover, the biological interface (micellar environment) showed to be an important parameter for the assessment of ACV controlled release.

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References

[1] A. J. Sawdon and C. Peng, Colloids Surf. B: Biointerfaces, 8 (2014) 738-745.
[2] J. W. Gnann, N. H. Barton and R. J. Whitley, Pharmacotherapy (1983) 275-283.
[3] M. Parsa, M. Javad, M. S. H. Reza, D. Simin, E. S. Ahmed, B. Bahram and H. Azadeh, Pharmacophore, 5 (2014), 483–493.
[4] M. Kubbinga, M. A. Nguyen, P. Staubach, S. Teerenstra and P. Langguth, Pharm. Res., 32 (2015) 2241–2249.

Smart drug delivery systems for cancer therapy

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Cancer remains a global health problem and a major cause of death worldwide. Statistical analysis published by the International Agency for Research on Cancer from the World Health Organization reveals that if the estimated trends continue, the incidence of all cancer cases will raise from 12.7 million new cases in 2008 to 21.2 million by 2030 [1]. Ideal nanocarrier-based therapy, contains first a controlled mechanism for drug delivery, to minimize side effects in healthy tissues, and second has the ability to provide a controlled drug release to extend the therapeutic duration of the therapeutic treatment.

Nanocarrier based chemotherapy is one of the few nanotechnology-based medical therapies that reached the clinics, already in 1995, when the commercial anticancer drug delivery system DOXIL® was introduced in the market [2], but available systems are far from optimal selectivity and controlled release.

Our work describes a combined spectroscopy and imaging study to evaluate a smart drug delivery system for cancer therapy. In our study we used DODAX:MO (1:2) formulations with a diameter of approx. 100 nm to study the biophysical characteristics when used for trafficking paclitaxel (PTX) and doxorubicin (DOX), both widely used chemotherapeutic anti-cancer drugs.Besides established biophysical profiling techniques to determine the pharmacokinetic of drugs; fluorescence based quenching assays allow a nanoscale localization of the anticancer drugs within the 100 nm diameter liposomal formulations.

In addition to the determination of the partition coefficients and the characterization of drug effects in membrane microviscosity, we use fluorescence (lifetime) spectroscopy to obtain nanoscale information of drug binding inside of innovative lipid based nano drug delivery systems, using molecular markers that are anchored at different depths within the lipid bilayer to sense the localization of the drug via a fluorescence quenching effect. To follow the internalization of liposomes into cancer cells we perform confocal fluorescence imaging of cancer cells exposed to liposomal formulations and compare with non encapsulated anticancer drugs.

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References

[1] F. Bray, A. Jemal, N. Grey, J. Ferlay, and D. Forman, The Lancet Oncology, 13 (2012) 790-801.

[2] Y, Barenholz, Journal of Control Release, 160 (2012) 117-134.

Pyrene as fluorescent probe of graphene in aqueous and micellar SDS dispersions

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Graphene, G, is the best known two-dimensional material, consisting of sp^2-hybridized carbon atoms arranged in a honeycomb lattice, and its properties make it very attractive in electronics, electromagnetic shielding, barrier coatings, composites, energy storage, sensing and other applications [1-2]. For a graphene dispersion to be useful, the nanomaterial should be dispersed in a suitable concentration, in an appropriate solvent, and with good kinetic stability. The presence of surfactants, stabilizing molecules of the dispersion, minimizes the free surface energy by non-covalent functionalization, avoiding the aggregation of the graphene sheets [3-4].

In this communication, we present the fluorescence behaviour of pyrene in dispersions of graphene in aqueous SDS solutions (below and above the CMC of SDS). Different graphene-to-surfactant weight ratios were used ranging from 0.5 to 2%. The exfoliation degree of the graphene sheets was examined by transmission electron microscopy (TEM) and Raman spectroscopy. Fluorescence quenching of pyrene was observed for all the dispersions although the data were well fitted to the Stern-Volmer equation for dispersions of graphene in micellar solutions. An ANOVA test (α=0.05) showed that there were no statistically significant differences in the values of the quenching constant for graphene dispersions in which SDS micelles were present, independently of the content of G. A value of $0.042 \pm 2x10^{-3}$ L mg^{-1} was obtained for the quenching constant.

Acknowledgements
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References
[1] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, Science, 306, (2004) 666-669.
[2] V. Singh, D. Joung, L. Zhai, S. Das, S.I. Khondaker, S. Seal, Prog. Mater. Sci., 56 (2011) 1178-1271.
[3] J. Texter, Curr. Opin. Colloid Interface Sci., 19 (2014) 163-174.
[4] R. Narayan, S.O. Kim, Nano Convergence (2015), 2:20 http://link.springer.com/article/10.1186/s40580-015-0050-x?view=classic

Importance of the hydrophobic interactions in the DNA compaction ability of surfactants

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Cationic surfactants have been successfully employed to interact with negatively charged biomolecules, such as proteins and nucleic acids. One of the most extensively studied applications of cationic surfactants regards to their use in gene therapy, as nucleic acid delivery systems [1]. It is based on the strong attractions between DNA and cationic surfactant aggregates. The current view is that both electrostatic and hydrophobic interactions play significant roles in the interactions of DNA with surfactants. The binding of the surfactant to the polynucleotide is a cooperative process associated with the self-assembly of the surfactant. In the presence of DNA the self-aggregation of the surfactant starts at a surfactant concentration much lower than the critical micelle concentration at which the surfactant form aggregates in the absence of DNA. However, to the authors´s knowledge, the DNA-surfactant interactions have not been tried to be fitted in a general way. In this work, for a group of surfactants with a 1+ charge, dodecyl chains and the same counterion, the importance of the hydrophobic interactions in the formation of the DNA:surfactant complex is shown through the linear dependence found when plotting the value of the molar ratio X=[surfactant]/[DNA] corresponding to the inflection point of the sigmoidal dependence of I/I_o on surfactant concentration vs. the surfactant cmc. I and I_o are the emission intensities of an aqueous solution of DNA and ethidium bromide in the presence and in the absence of surfactant, respectively. A similar linear dependence is also found between the molar ratio X at which the ξ-potential of the DNA:surfactant complex is zero, usually called the isoneutrality ratio, and the surfactant cmc.

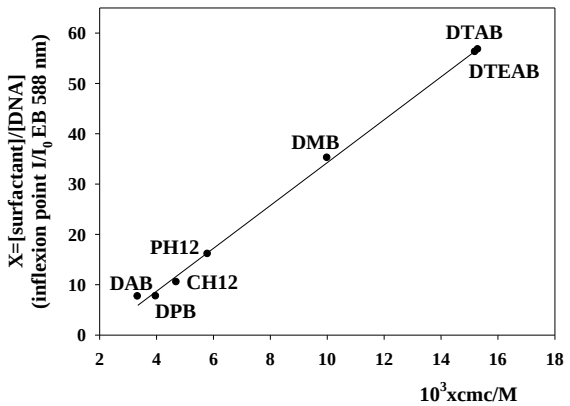

Figure 1.-Dependence of the X(inflexion point of I/I_o vs. [surfactant]) on the surfactant cmc.DTAB:Dodecyltrimethylammonium bromide; DTEAB:Dodecyltriethylammonium bromide; DMB:Dodecylimidazolinium bromide; PH12:N-benzyl-N,N-dimethyl-N-(1-dodecyl)ammonium bromide; CH12:N-cyclohexylmethyl- N,N-dimethyl-N-(1-dodecyl)ammonium bromide; DPB:Dodecylpyridinium bromide; DAB:[2-(2-benzoilamino-etoxy)ethyl]-*N*-dodecyl-*N*,*N*-dimethyl-ammonium bromide.

Additional studies are being carried out involving surfactants with the same head group and counterions, but different hydrophobic tail lengths. The influence of the nature of the counterions as well as the number of hydrophobic chains will also be investigated. The goal is to investigate if similar correlations are found in all cases.

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References
[1] M. Mishra, P. Muthuprasanna, K. S. Prabha, P. S. Rani, I. A. S. Babu, I. S. Chandiran, G. Arunachalam, S. Shalini, Basics and potential applications of surfactants-A review. Int. J. PharmTech. Res. 1 (2009) 1354−1365.

The concerted action involving conformation and desolvation that makes water-soluble bambusurils unique anion cages

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Anion containers have a key role in a variety of systems with technological and biological relevance, in which they have been linked to diseases related to ion channels in the muscle, bone and brain. In these systems, compatibility with aqueous media is mandatory. However, water may hinder the binding affinity in molecular recognition, thus fostering the development of new host-anion systems.[1] Water-soluble bambusurils (BUs) can bind and isolate inorganic anions in the center of the hydrophobic cavity, with high affinity and selectivity.[1] This makes them appealing anion carriers and ion transporters for a wide range of biomedical applications. For understanding the bambusuril ion caging ability in aqueous media, molecular dynamics (MD) simulations, including free energy calculations are used.[2] The new computational studies reveal for the first time relevant aspects related to the conformation, hydration and binding behavior of three bambusurils. Particularly, the complexation of the water-soluble derivative containing twelve benzoyl groups, $(BnCOOH)_{12}BU[6]$, with chloride ions is inspected in detail. The $(BnCOOH)_{12}BU[6]$ conformation varies significantly in the absence of the chloride ion, i.e., collapsed structures frequently occur. Upon formation of the inclusion complex with chloride, collapse is prevented. The ion is hermetically sealed inside the cavity, as a result of a concerted action involving conformation and desolvation of both ion and bambusuril cavity. It is also relevant to point out that complete desolvation of the anion is observed in this system, with a cavity being closed by the substituent groups, and thus isolated the interior from the bulk water. Simulations conducted with other substituted bambusurils indicated that the water occupancy in the cavity, and in the absence of included ions, varies significantly with the type and size of the substituents. In some cases, there are indications that the collapse of the cavity may be the factor governing water occupancy. From the theoretical perspective, computer simulations of the systems involving bambusurils, employing systematic approaches, are almost inexistent and are clearly useful to predict and guide future studies. The variety of possibilities related to the number and type of host and guest molecules suggests that a systematic rationalization of the inclusion complexes is most relevant.

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References
[1] T.F.G.G. Cova, S.C.C. Nunes, T. M.V.D. Pinho e Melo,A.A.C.C. Pais.*Chem. Phys. Lett*. 672 (2017) 89-96;
[2]T.F.G.G. Cova, S.C.C. Nunes, A.A.C.C. Pais, *Phys. Chem. Chem. Phys*. 19 (2017) 5209-5221.

Cellulose as a dispersion stabilizer

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Important stabilizers of disperse systems are polymers with amphiphilic properties. Here cellulose derivatives have an important position and methyl cellulose (MC), ethyl cellulose (EC), ethylhydroxyethyl cellulose (EHEC) and hydroxypropyl methyl cellulose (HPMC) are well known as efficient stabilizers in emulsions. This highlights their amphiphilic nature, which is clearly not only an effect of the different chemical modifications but it must reside in the native cellulose backbone. In arguing that cellulose itself should be considered as an amphiphilic polymer, cellulose would be expected to locate at the oil-water interfaces and thus act as a good stabilizer in an emulsion; as well as other disperse systems (like foams). The use of native cellulose without the need of chemical modifications represents a clear advantage for developing biocompatible, biodegradable and nontoxic formulations. Aqueous-based solvents are the most important class for dissolving cellulose in a first step, since the water used for dissolution can remain as either the dispersed phase or the dispersion medium in the final emulsion, otherwise any other solvent would need to be removed involving a more complex process. In this work cellulose adsorption and its interfacial activity will be highlighted. Emulsions formed by native cellulose are further characterized by droplet's size and size distributions and long-term stability.

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Hydrophobically-modified chitosan nanovectors for efficient siRNA delivery

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The RNA interference (RNAi) constitutes a conservative mechanism in eukaryotic cells that induces silencing of target genes. In mammalians, the RNAi is triggered by siRNA (small interfering RNA) molecules. Due to its potential in silencing specific genes, the siRNA has been considered a potential alternative for the treatment of genetic and acquired diseases [1]. However, the use of siRNA is hampered by its rapid degradation and poor cellular uptake into cells *in vitro* or *in vivo*. Therefore, we have explored hydrophobic modified chitosan as a siRNA vector due to its advantages such low toxicity, biodegradability and biocompatibility [2-3]. This study aims at developing of cross-linked chitosan nanoparticles suitable for an intravenous administration of small siRNA able to achieve high gene silencing without cytotoxicity, stability at physiological pH and long storage time stability. Chitosan nanoparticles were prepared by ionic gelation using sodium tripolyphosphate (TPP). This nanoparticles exhibited a mean hydrodynamic diameter of 190 nm with a polydispersity index (PDI) of 0.126 and a zeta potential of +36 mV, high binding capacity, loading efficiency and nanoparticles had good storage stability at room temperature up to at least 15 days. *In vitro* studies in HeLa/GFP cell line revealed that hydrophobic modification of chitosan improves cellular uptake and long term siRNA release into cytoplasm. Therefore, our chitosan nanoparticles system show much potential as viable vector for safer, high efficient and low-cost siRNA delivery.

Acknowledgements
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References
[1] K. A. Whitehead, R. Langer, D. G. Anderson, Nature Rev. Drug Discov. 8 (2009) 129-128.
[2] J. E. Zuckerman, M. E. David, Nature Rev. Drug Discov., 14 (2015) 843-856.
[3] R. Kanasty, J. R. Dorkin, A. Vegas, D. Anderson, Nature Mater., 12 (2013) 967-977.

Synthesis and characterization of protein-loaded nanocapsules

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Nanotechnology can improve diagnostic and therapeutic procedures such as drug delivery and cancer treatment [1].Polymeric particles and capsules are being widely studied as exceptional carriers in such applications thanks to their intended biocompatibility and potential biodegradability, selective acummulation in the disease area and their ability to encapsulate and release in a controlled fashion a wide range of bioactive compounds, among other relevant bioproperties [1].
In the present work, calcium carbonate nanoparticles ($CaCO_3$ NPs) were synthesized by combining Na_2CO_3 and $CaCl_2$ in the presence of poly (vinylsulfonic acid) (PVSA). The $CaCO_3$ NPs were loaded with FITC-bovine serum albumin (BSA) labeled (FITC, fluorescein isothiocyanate), as a model cargo. Then, calcium carbonate cores were coated with oppositely charged polyelectrolytespoly(sodium 4-styrenesulfonate) (PSS) and poly(diallyldimethylammonium chloride) (PDADMAC) as negative and positive polyelectrolytes, respectively. Finally, the sacrificial inner core was dissolved in order to fabricate the polymeric nanocapsules. The morphology of the nanocapsules in each fabrication step was characterized by dynamic laser-light scattering (DLS), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and UV-Vis Spectroscopy. In summary, the average nanocapsule sizes were found to be in the range of ca. 200 – 1000 nm. Furthermore, a reversal of the surface electrical charge between positive and negative zeta potential values was found, proving the layer-by-layer deposition was successful. The protein leakage was monitored during one week through UV-Vis spectroscopy and thet stability of the capsules in different bioligically relevant micmicking media.

Acknowledgements
This work was supported by AEI and ERDF through projectsMAT2015-74381-JIN and MAT2016-80266-R.

References
[1] S. Hinderer, S. Lee-Layland, K. Schenke-Layland, Adv. Drug Deliv. Rev., 97 (2016) 260-269.
[2] M. Elsabahy, G. S. Heo, S.-M. Lim, G. Sun, K. L. Wooley, Chem. Rev., 115 (2015) 10967-11011.

Evaluation of activity and degradation in biological media of upconverting-based nanoplatforms for theranostic applications

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Recent advances in biomedicine are oriented to combine therapy and diagnosis in an efficient way. Upconverting nanoparticles (UCNPs) are a relatively novel type of nanoparticles (NPs)with outstanding properties which allow to overcome some of the main disadvantages of other nanomaterials currently analyzed nowadays for theranostic applications [1]. The main characteristic of UCNPsis their luminiscence when excited by near-infrared (NIR) radiation and subsequent energy emission in the form of visible and ultraviolet light through anti-Stokes processes [2] being,then, their activation wavelength within the so-called biological window. The luminiscent light emitted by UCNPscan be exploited to stimulate many photosensitizers (PS) which, upon excitation,generate cytotoxic reactive oxygen specicies, the basis of photodynamic therapy (PDT) [3]. Moreover, the emitted light by UCNPs can be also used for high resolution optical imaging, and when incorporating gadollinium either in the matrix core or within the NP shell, additional capabilities of T_1 magnetic resonance imaging (MRI) contrast agent can be incoporated within a single UCNP. In this work, we have synthesized UCNPs with different compositions and dopants, analyzing their effect on particle size, shape and luminiscent properties.As the as-synthesized UCNPs are hydrophobic, a ligand exchange process with different ligands have been performed to achieve perfect dispersability and stability in biological-mimicking media. In addition, PSs as Rose Bengal and/or Chlorin e6 were attached to the NPs and the PDT activity of the created nanoplatform was elucidated. In vitro studies were performed in order to test the cytotoxic activity of the nanoplatform, their internalization and degradation process inside severla tumoral cell lines.

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References
[1] M. Nichkova , D. Dosev , S. J. Gee , B. D. Hammock, I. M. Kennedy. Anal. Chem., 77 (2005) 6864-6873.
[2] F. Auzel. Chem. Rev., 104 (2004) 139-173.
[3] L. Cheng, C. Wang, L. Feng, K. Yang, Z. Liu. Chem. Rev., 114 (2014) 10869-10939.

Two-dimensional self-assembled arrays of metallic nanoparticles for biotechnological applications

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In the last few years, an important effort to design and obtain new optical (bio)sensors with applications in diverse disciplines like biomolecular sensing, clinical diagnosis, environmental control and food industry as been performed. Different studies [1] have shown that ordered (quasi)arranged patterns composed of anisotropic shape metal nanoparticles provide significant increases of the Raman signals of analytes due to the enhancement of the electromagnetic field at certain regions within/between the interacting metallic nanostructures [2] (the so-called ‘‘hot spots’’[3]). Therefore, there substrates can be potential good candidates to be used as SERS (bio)sensors. In order to build up these nanosensors, the use of block copolymer litography (BCL) is very attractive because of the spontaneous auto-organization of the block copolymer domains in the nanoscale, which allows the parallel large-scale production of periodic metallic nanostructures at low cost and very efficiently.
Thus, this work has been focused on obtaining bimetallic plasmonic substrates using BCL to achieve 2D well-ordered gold nanoparticles patterns used as seedsfor a subsequent growth process. In this manner, we generate quasi-hexagonal ordered arrays of star-like gold core/silver shell nanoparticles with controllable core size and shell thickness, and interdistances. These substrates exhibit SERS enhancement properties tested by detection of different food contaminants like phthalates and melamine. We also probed theirprotential use as photothermalheaters underfar-Vis/near infrared illumination and the evolution on the array/particle structure under different illumination conditions in order to determine the potential release of Ag ions to the medium with potential antimicrobial activity.

Acknowledgements
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References
[1]V. López-Puente, S. Abalde-Cela, P. C. angelomé, R. A. Alvarez-Puebla, L. M. Liz-Marzán, J. Phys. Chem. Lett. 4 (2013) 2715-2720.
[2] L. Tong, T. Zhu, Z. Liu, Chem. Soc. Rev. 40 (2011) 1296-1304.
[3] R. A. Alvarez-Puebla, L. M. Liz-Marzan, Small, 6 (2010) 604-610.

Studies on the interaction of cationic polymers with microorganisms: development of photobactericidal surfaces

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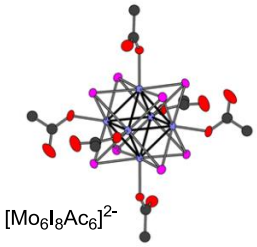
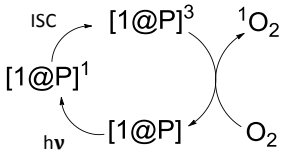
The formation of bacterial biofilms on the surface of materials is becoming a serious health problem taking into account that this kind of accumulation of microorganisms is extremely resistant to conventional disinfection methods [1]. Increasing attention is currently devoted to the development of surfaces disfavouring the adhesion of bacteria and hence impeding the formation of biofilms. One of the strategies consists in the use of cationic groups able to disrupt the membrane of the microorganism (alkylamonium, phosphonium, sulfonium, etc) [2]. Another strategy to fight bacterial infections is the antimicrobial photodynamic therapy (aPDT), which makes use of a photosensitizer to generate cytotoxic reactive oxygen species, such as singlet oxygen ($^1O_2$) [3].



Cluster 1



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In this communication we have combined both strategies in order to develop a series of materials with cationic groups at the surface and containing a new photosensitizer displaying great efficiency for the generation of $^1O_2$ (complex $[Mo_6I_8Ac_6]^{2-}$) [4]. It has been found that the nature of the polymeric matrix (macroporous vs gel-type) has a profound influence on the photobactericidal properties of the studied materials. Photoinduced killing of both gram-positive Staphylococcus aureus and gram-negative Pseudomonas aeruginosa have been found [5].

References

[1] K. Page, M. Wilson and I. P. Parkin, J. Mater. Chem., 19 (2009) 3819-3831.
[2] D. Campoccia, L. Montanaro and C. R. Arciola, Biomaterials, 34 (2013) 8533-8554.
[3] C. Spagnul, L. C. Turner and R. W. Boyle, J. Photochem. Photobiol. B: Biol., 150 (2015) 11-30.
[4] M. A. Mikhailov, K. A. Brylev, P. A. Abramov, E. Sakuda, S. Akagi, A. Ito, N. Kitamura and M. N. Sokolov, Inorg. Chem., 55 (2016) 8437-8445.
[5] A. Beltrán, M. Mikhailov, M. N. Sokolov, Vanesa Pérez-Laguna, A. Rezusta, M. J. Revillo and F. Galindo, J. Mater. Chem. B., 4 (2016) 5975-5979.

Deamidation of pseudopeptidic supramolecular gels and its application to controlled release

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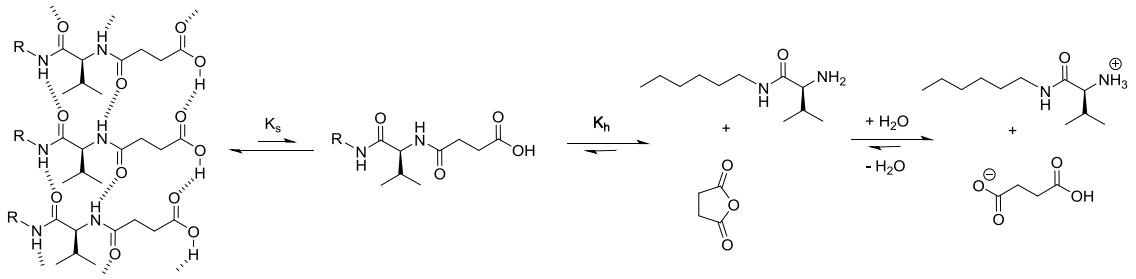
The study of gel formation by peptides and related motifs has received especial attention due to the biological relevance of protein and peptide aggregation. [1] Following our studies in the kinetics and thermodynamics of aggregation of peptide-related compounds [2] here we report on how supramolecular hydrogels formed by pseudopeptidic derivatives of L-valine suffer a thermal deamidation reaction, leading to partial disassembly.

The succinic acid-derived moiety present in the gelators is responsible of intramolecular catalysis of a deamidation reaction. Such neighboring group effect is reminiscent of biochemical processes such as protein deamidation and self-excision of inteins. It has been found that the thermodynamic equilibrium of the deamidation reaction is regulated by the efficiency of hydrogelation. As a proof of concept, the thermally promoted deamidation is applied to controlled release of Rose Bengal.



Acknowledgements
Ministerio de Economía y Competitividad of Spain (CTQ2015-71004-R) and Universitat Jaume I (P1.1B2015-76) are thanked for financial support.

References
[1] I. W. Hamley, Angew. Chem. Int. Ed., 46, (2007), 8128-8147.
[2] M. Tena-Solsona, J. F. Miravet and B. Escuder, Chem. Eur. J., 20, (2014), 1023-1031.

Surface properties of conducting polymer films

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In recent years, conductive polymers have attracted important attention for their potential applications as components of light emitting diodes, polymer solar cells and sensors [1, 2]. The excellent optoelectronic properties of that kind of polymers have been interpreted as owing to the formation of nanofibers which highly increase the conductivity and they do not diminish the optical transparency. The polymer nanofibers are formed by polymer chain association throwing π-π interactions that mainly depends on the temperature and concentration when the polymer chains are dissolved in poor solvent [2]. On the other hand, for manufacturing transparent conducting electrodes using these polymers nanofibers can be transferred to Si-SiO_2 wafer by the drop-cast methodology [3]. This methodology often renders undesirable processes due to hydrodynamic and capillary phenomena; therefore we propose a more adequate transfer methodology such as Langmuir-Blodgett or Langmuir-Schaefer Methodologies as alternative techniques. These deposition methods allow a great control on the film morphology and were successfully used to prepare thin films of silver nanowires [4], semiconductor Quantum Dots [5] and graphene derivatives [6].

Accordingly, we explore the ability of the air-water interface to promote the aggregation of the Poly (3-hexylthiophene) or P3HT by analyzing the surface pressure and potential-area isotherms of the conductive polymer at the air-liquid interface. The next step was to transfer the polymer aggregates from the air-water interface to the solid wafer (Si/SiO2) by the Langmuir Blodgett Methodology. Finally, we analyze the film morphology by SEM and we determine the electric conductivity.

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References
[1] W. Dierckx, W. D. Oosterbaan, J-C Bolseé, W. Maes, D. Vanderzande and J. Manca, J. Mater. Chem. C, 2 (2014) 5730-5746.
[2] S. Berson, R. De Bettignies, S. Bailly and S. Guillerez Adv. Funct. Mater. 17 (2007) 1377-1384.
[3] Y. Guo, L. Jiang, X. Ma, W. Hu and Z. Su, Polym. Chem., 4 (2013) 4308-4311.
[4] D. López-Díaz, C. Merino and M.M. Velázquez, Materials, 8 (2015) 7622-7633.
[5] T. Alejo, M.D. Merchán, M.M. Velázquez and J.A. Pérez-Hernández, Mat. Chem. Phys., 138 (2013) 286-294.
[6] R.S. Hidalgo, D. López-Díaz and M.M. Velázquez, Langmuir, 31 (2015) 2697-2705.

Surface properties of Nanocomposites for capturing of CO_2

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The discovery of novel materials with large storage capacity of carbon dioxide and the possibility of being recycled is a very important challenge in order to reduce the emissions of heating gases. Several methodologies, such as chemical fixation with aqueous solutions containing amines, adsorption onto silica, zeoliteshave been proposed. The main problem of using amines is the prohibitive cost while in the case of inorganic materials degradation upon regeneration is a disadvantage.

Owing to the exceptional adsorption properties and low energy requirements for regeneration, carbon based materials (activated carbon and carbon nanofibers or nanotubes) are considered to be one of the most promising materials for capturing carbon dioxide. Recently, Graphene Oxide (GO) have been also proposed as good candidate, however its efficiency as CO_2 adsorbent must be improved. An alternative is to prepare composites based on GO which is normally synthetized by means of the Staudenmaier or the Hummers methods. The presence of oxygen functional groups introduced during the chemical oxidation allows attaching polymers or nanoparticles. An important issue which is not taking into account in these studies is that the chemical composition changes depending on the starting material and oxidative protocol employed to GO synthesis. Therefore, in this work, we have studied the effect of the chemical composition of GO on the adsorption properties of nanocomposites of polyaniline or magnetite nanoparticles and GO. For this purpose, GO of different chemical compositions were synthesized by oxidation of graphite and GANF carbon nanofibers [1] [2][3] and then were used to obtain nanocomposites with polyaniline and magnetite

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Authors thanks Junta de Castilla y Leon (SA045U16) and MINECO (CTQ2016-78895-R) for funding the research.

References
[1] López-Díaz D, Velázquez M M, et al. ChemPhysChem. 14, 4002-4009, 2013.
[2] Martín-García B, Velázquez M M, et al. ChemPhysChem. 13, 3682-3690, 2012.
[3] Hidalgo R S, López-Díaz D, et al. Langmuir. 31, 2697-2705, 2015.

Control over phase synchronisation in rotor models of motile cilia

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The coordinated cyclic beating of eukaryotic cilia and flagella is responsible for vital functions such asmotility of microorganisms and fluid transport close to various epithelial tissues. Synchronizationinduced by hydrodynamic interactions is a possible and potentially general mechanism behind thiscoordinated beating of cilia. To understand hydrodynamic synchronization, rather than a realisticbeating filament description, we use here a simple model with a minimal number of degrees offreedom, based on optically driving a pair of colloidal particles, [1, 2] that act as micron-scale phaseoscillators. Intra-cilia properties are thus coarse grained into the parameters chosen to drive theparticles around closed orbits. We show that different phase-locked steady states –forinstance, In-Phase or Out-of-Phase– can be achieved depending on these parameters, and present a regime diagram. Modest tuning of the cilia beating properties, as could be achieved biologically by modulation themolecular motor activity or binding affinity, or the cilia length and orientation, can lead to dramaticchanges in the collective motion that arises out of hydrodynamic coupling. The experimental resultsare consistent with analytical calculations that include the driving force and the hydrodynamicinteraction. [3]

References

[1] J. Kotar, L. Debono, N. Bruot et al, *Phys. Rev. Lett.***111**, (2013), 228103.

[2] N. Uchida and R. Golestanian, *Phys. Rev. Lett.***106**, (2011), 058104.

[3] A. Maestro, N. Bruot, J. Kotar, et al. Submitted.

PLGA nanoparticles for delivery of Bone Morphogenetic Protein and biofunctionalization of Titanium surfaces

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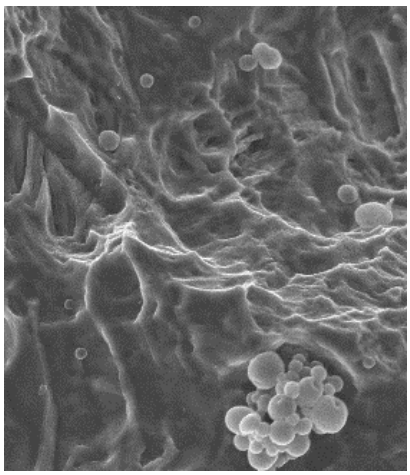
Nanoparticles (NPs) based on the polymer Poly (lactide-co-glycolide) acid (PLGA) have been widely studied for the development of delivery systems for drugs and therapeutic biomolecules,due to the biocompatible and biodegradable properties of the PLGA. In this work, a synthesis method for Bone Morphogenetic Protein (BMP2)-loaded PLGA NPs has been developed and optimized, based on the double-emulsion (water/oil/water, W/O/W) solvent evaporation technique. The polymeric surfactant Pluronic F68 was used in the synthesis procedure, as it is known to have an effect on the reduction of the size of the NPs, the enhancement of their stability, and the protection of the encapsulated biomolecule, together with the fact that its presence on the surface of the NPs reduces their recognition by the mononuclear phagocytic system. Spherical hard NPs were obtained, showing a reproducible multimodal size distribution with diameters between 100 and 500 nm. This range of sizes would allow the protein to act at cell surface and cytoplasm level. The colloidal properties of these systems (morphology by SEM and STEM, hydrodynamic size, electrophoretic mobility, temporal stability, protein encapsulation and release) were studied. These NPs were also linked to a Titanium surface via Dopamine. The effects of the free and linked BMP2-loaded NPs on Human Mesenchymal Stem Cells were also analyzed *in vitro*.



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References

G.E.J. Poinern, *A laboratory course in nanoscience and nanotechnology*, 2015, Chapter 5, 140-146, CRC Press, Taylor & Francis Group, London, UK.

I. Ortega-Oller, M. Padial-Molina, P. Galindo-Moreno, F. O´Valle, A.B. Jódar-Reyes, J.M. Peula-García, *BiomedResearch International*, 2015, Article ID 415289.

Farace, C., Sánchez-Moreno, P., Orecchioni, M., Manetti, R., Sgarrella, F., Asara, Y., Delogu, L. G. (2016). Immune cell impact of three differently coated lipid nanocapsules: pluronic, chitosan and polyethylene glycol. Scientific Reports, 6(1), 18423.

White, L. J., Kirby, G. T. S., Cox, H. C., Qodratnama, R., Qutachi, O., Rose, F. R. A. J., & Shakesheff, K. M. (2013). Accelerating protein release from microparticles for regenerative medicine applications. Materials Science and Engineering: C, 33(5), 2578–2583.

Optimized surfactant/polymer interactions for the improvement of detergent efficiency

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The interaction between polymers and surfactants and its impact on foam formation and stability, emulsification power and enzymatic catalytic activity were evaluated by circular dichroism, enzyme activity determination, foam formation and emulsification index (the system should be introduced here).

The work is divided into two parts. Firstly the conformational changes and the enzymatic activity of a protein in the presence of model surfactants, sodium dodecyl sulfate, (SDS also denoted as SLE_0S) and sodium lauryl ether sulfate with two ethylene oxide (EO) units (SLE_2S), were studied.Secondly, thefoam formation, their stability and the capacity ofoil emulsificationin systems containing a hydrophobically modified linear polymer and a combination of SLE_1S and SLE_2S were assessed.

The results strongly suggest that the presence of EO units in the surfactant polar headgroup determines the stability and the activity of the enzyme. SDS promotes enzyme denaturation and consequent loss of activity, while the SLE_2S preserves the enzyme structure and activity. Moreover, data suggests that the ideal ratio between hydrophobically modified linear polymers and surfactants wasthe most effective parameter to control foam stability. Due to polymer positioning at the foam droplets/bubbles interfaces, this leads to high viscosity of the liquid phase which avoids the bubbles from bursting. Regarding the emulsification, the more efficient systems were the ones containing polymer and surfactant which are capable to produce relatively long living emulsions.

These results show that the tuning the interactions between polymers and surfactants may lead to detergents with improved performance.

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Study of phase separation in a negatively charged colloid / polymer system

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Colloidal dispersions composed by mixtures of particles and non-adsorbent polymers separate into two distinct thermodynamic phases at certain particle-to-polymer ratios; this is due to a depletion force, generated by the polymer, which induces an attraction between colloidal particles, and thus their ultimate aggregation [1]. When both components are negatively charged, this phase separation occurs at lower concentrations of the components; this is likely due to the emergence of an ionic force that acts synergistically with the depletion force responsible for the phase separation observed in neutral dispersions. Nevertheless, the ionic force may lessen the depletion interaction due to a decrease of the ionic lenght of the particles [2]. To demonstrate this hypothesis, here we present data on the kinetics of the phase separation and on the mechanical properties of each thermodynamic phase. In particular, we show that the lower the concentration of polymer, the faster the phase separation. Moreover, the rheological study shows that the phase rich in particles has a high elasticity, and that the elasticity of this phase increases with polymer concentration, while the particle aggregates become more breakable. This study may help explain the posible consequences of overlapping depletion and ionic forces when designing coloidal systems for different applications.

Acknowledgements
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.References
[1] Asakura, S., & Oosawa, F. (1954). The Journal of Chemical Physics, 22(7), 1255.
[2] Peláez-Fernández, M., Moncho-Jordá, A., & Callejas-Fernández, J. (2010). Europhysics Letters, 90(4), 46005

Hyaluronic Acid-Human Serum Albumin (HAS) Complexes at Fluid Interfaces

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Liquid lipid nanocapsules (LLNs) are colloidal systems consisting of a liquid lipid core surrounded by an amphiphilic protective shell[1] and represent a novel promise as drug delivery systems . LLNs constitute a new generation of nanoparticles with a higher degree of biocompatibility and versatility, especially when they are prepared with natural materials that possess the biocompatibility, biodegradability, and non-toxicity required for use in humans. Hyaluronic Acid (HA) is a natural compound whichis being used in targeted delivery of drugs on the tumour cell through its selective binding to an specific receptor, CD44 [2]. hence, in order to optimise performance of LLN, the protective shell should contain (HA) combined with other bioactive molecules such as Human Serum Albumin (HSA). The interfacial properties of HA, HSA and interfacial complexation is expected to play an important role in the rational design of LLN. In this work we show a detailed interfacial characterization of HA adsorbed layers at fluid interfaces and the interfacial activity of HA-HSA complexes. The objective is to understand the interfacial phenomena underlying degradation and stability of LLN with the aim of optimizing the preparation and performance of these nanocarriers.

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References:

1. J.A. Molina-Bolívar, F. Galisteo-González, Olive-oil nanocapsules stabilized byHSA: influence of processing variables on particle properties, J. Nanopart. Res. (2015) **17**, 1–13.
2. K. Y. Choi, G. Saravanakumar, J. H. Park, K. Park, Colloids and Surfaces B: Biointerfaces (2012) **99** 82– 94.

Surfactant-assisted exfoliation of graphite into graphene: dispersibility studies and structural characterization

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In recent years, graphene has become an exciting nanomaterial for a wide range of applications. Because of graphene's insolubility in aqueous media, surfactants are often used to stabilize the exfoliated material, owing to the electrostatic or steric repulsions provided by the adsorbed amphiphile [1,2]. In this work, we have developed and explored a methodology to exfoliate graphite in aqueous surfactant solution under well-controlled conditions. From the profile of the dispersibility curve, several quantitative parameters were extracted, which altogether permit reliable comparisons between different surfactants [3-5]. Further, the exfoliated material was characterized by AFM and SEM, allowing the determination of the content of few-layer graphene in the dispersions. Thus, this work contributes to a systematic investigation on the mechanisms of surfactant-assisted exfoliation of graphite, establishing a robust methodology to control the variables of the process and hence study the effect of specific molecular parameters that may lead to dispersal optimization.

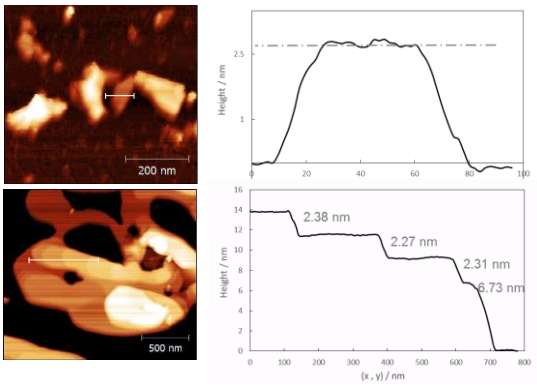

Figure 1.AFM micrographs and height profile of: (top) nominal monolayer and (bottom) terraces of a graphene flake.

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References
[1] L.P. Biró, P. Nemes-Incze and P.Lambin. Nanoscale 4.6 (2012) 1824-1839.
[2] R. J. Smith, M. Lotya, and J. N. Coleman, New J. Phys., 12 (2010) 125008.
[3] R.M.F. Fernandes, B. Abreu, B. Claro, M. Buzaglo, O. Regev, I. Furo and E.F. Marques, Langmuir, 31 (2015) 10955-10965.
[4] M. Buzaglo, M. Shtein, S. Kober, R. Lovrinčić, A. Vilan and O. Regev, Phys. Chem. Chem. Phys., 15 (2013) 4428-4435.
[5] M. Shtein, I. Pri-Bar, M. Varenik and O. Regev, Anal. Chem., 87 (2015) 4076-4080.

Bioreducible polycation-DNA complexes

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The delivery of genes for therapeutic applications requires advanced nanocarriers that can package and protect DNA, and then deliver it to ill cells or tissues. Polyplexes – soft nanoparticles resulting from the complexation of DNA with cationic polymers – are promising vehicles to achieve these goals, but further advances in the technology are needed to achieve the desired efficiency for use in gene therapy applications [1].

One promising approach to enhance the gene delivery efficiency of these particles employs the use of polycations with disulfide bonds along their backbone that degrade in the reducing potential of the cytosol. This leads to an enhanced release of genes inside cells, and lowers the toxicity of the polymer [2].

In this work, we test different assembly pathways with and without the presence of physiological buffer, and rationalize their influence in the structure, size and charge of bioreducible polyplexes. This is an important first step that will later facilitate the establishment of relations between the structure of the particles and their efficiency in delivering the genes in cells, and allow the design of more efficient polyplexes with potential for therapeutic applications.The main characterization techniques used were Dynamic Light Scattering (DLS), Zeta Potential, Small-angle X-ray Scattering (SAXS) and cryo-TEM.

Acknowledgements
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References
[1] Lachelt, U. and E. Wagner, 115 (2015) 11043-78.
[2] Oupicky, D. J. Li, 14 (2014) 908-22.

Raman studies on graphene-based materials doped with metal sulfides

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Graphene based materials have emerged as promising materials in many technologies due to their structure dependent physical and chemical properties [1]. Metal chalcogenide nanocrystals have also attracted great attention because of their size-dependent properties and their potential application in diverse areas, which include sensors, solar cells, catalysts and optoelectronic devices [2]. However, there are few synthetic routes that result in morphological uniform hybrid materials comprising both components, which in some cases can be related to lack of knowledge about surface chemical effects on the synthesis itself. Hence, in this research we have studied the *in situ* growth of metal sulfide nanocrystals (Ag_2S, Bi_2S_3, CdS and PbS), in the presence of graphene oxideand exfoliated graphite oxide flakes dispersed in ethanol, by the thermolysis of the respectivemetal dialkyldithiocarbamate complex [3].

Several synthesis parameters have been investigated in order to optimize experimental conditions for obtaining morphological uniform hybrid nanomaterials. Raman spectroscopic methods have been applied to monitor the surface nature of carbon substrates due to their potential impact on the nucleation and growth of the metal sulfide nanophases onto the graphene-based surfaces.The hybrid nanostructures were also characterized for their morphological features using SEM and TEM.

Acknowledgements
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References
[1] A. Ciesielski and P. Samori, Chem. Soc. Rev., 43 (2014) 381-398.
[2]T. Trindade and P. J. Thomas, Defining and Using Very Small. Crystals, Comprehensive Inorganic Chemistry II: From Elements to Applications., J. Reedijk and K. Poeppelmeier; Elsevier, Oxford, England, 4 (2013) 343-369.
[3] A. C. Estrada, E. Mendoza and T. Trindade, Eur. J. Inorg. Chem., 2014 (2014) 3184-3190.

Towards a realistic modelling of protein diffusion in polymer crowded media

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The high concentration of macromolecules (*i.e.*, macromolecular crowding) in cellular environments leads to large quantitative effects on the dynamic and equilibrium biological properties [1]. Since in vitro experiments are usually carried out at low concentrations (1–10 g/L), alternative approaches are necessary in order to evaluate the effect of macromolecular crowding in the thermodynamic and kinetic properties of biological systems.

At the experimental level, high concentrations of crowding agents (usually Dextran or Ficoll macromolecules), which are considered to interact only by means of steric non-specific interactions, have been used to mimic the in vivo environment. The experimental studies of macromolecule diffusion are mainly based on two experimental techniques: Fluorescence Correlation Spectroscopy (FCS) [2] and Fluorescence Recovery After Photobleaching (FRAP) [3].

In addition, computational studies have been performed in order to understand the effect of macromolecular crowding. These studies use different approaches such as *on-lattice* Monte Carlo simulations [4-5] or *off-lattice* Brownian Dynamics (BD) simulations [6-8].

In the present work, a novel model for macromolecule diffusion in crowded media is presented. This model allows to effectively accounting for polymer entanglement and macromolecular folding in highly concentrated macromolecular solution. The results obtained are compared with previous experimental studies of protein diffusion in crowded media [8]. The study proposed reveals the relevance of polymer aggregation, polymer folding and hydrodynamic interactions to properly reproduce the experimentally observed diffusion behaviour.

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References
[1] Zhou, H.X., Rivas, G., Minton, A.P.,Annu Rev Biophys 37 (2008) 375.
[2] Banks, D.S.; Fradin, C. Biophys. J. 89 (2005) 2960.
[3] Pastor, I. , Vilaseca, E., Madurga, S., Garcés, J.L., Cascante, M., Mas, F., J. Phys.Chem. B 114 (2010) 4028 &*Erratum ibid* 114 (2010) 12182.
[4] Vilaseca, E., Isvoran, A., Madurga, S., Pastor, I., Garcés, J.L., Mas, F., PhysChem-ChemPhysm 13 (2011) 7396.
[5] Pitulice, L.; Vilaseca, E.; Pastor, I.; Madurga, S.; Garcés, J.L.; Isovran, A.; Mas, F., Mathematical Biosciences, 251 (2014) 72.
[6] Ermak, D.L., McCammon, J. A., J.Chem. Phys. 69 (1978) 1352.
[7] Tokuyama, M., Moriki, T., Kimura, Y., Phys. Rev. E, 83 (2011) 081402-1.
[8] Blanco, P.M.; Via, M.; Garcés, J.L.; Madurga, S.; Mas, F., Entropy, 19 (2017) 105.

Cationic lipid nanoparticles for topical drug administration

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Lipid nanoparticles are colloidal carriers, composed ofbiocompatible lipids, which have been used as attractive delivery systems for various drugs through several routes of administration [1, 2].

This work aimed at developing and optimizing a formulation based on nanostructured lipid carriers for topical administration of miconazole nitrate. Different lipid nanocarriers (LN) with various solid:liquid compositions were formulated and tested in terms of stability and incorporation capacity of miconazole nitrate. The lipid nanocarriers were formulated by the method of hot high pressure homogenization (HPH) which was used to prepare solid lipid nanoparticles (SLN), nanoemulsions (NE) and nanostructured lipid carriers (NLC). The pharmaceutical development included the selection of the type of lipid (solid and liquid) and surfactant, the solid/liquid lipid and internal/external phase ratios. Along the project, stability tests were performed in order to select the best formulation for a long-term storage. Finally, the results favora NLC-based formulation with 1% (w/w of total lipid content) of Didodecyl dimethyl ammonium bromide, a positive quaternary ammonium compound, and 0.25% (w/V) of miconazole nitrate as the most promising formulation in terms of stability (ZP>30) for topical delivery of miconazole nitrate.

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References
[1] Mendes, M., et al., Can lipid nanoparticles improve intestinal absorption? International Journal of Pharmaceutics, 2016. 515(1–2): p. 69-83.
[2] Vitorino, C., et al., Co-encapsulating nanostructured lipid carriers for transdermal application: From experimental design to the molecular detail. Journal of Controlled Release, 2013. 167(3): p. 301-314.

Serine based gemini lipid nanoparticles for glioblastoma treatment

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Glioblastoma multiforme (GBM) is the most common primary brain tumour, and the most aggressive in nature. Cationic nanostructured lipid nanoparticles (cNLCs) are an appealing drug nanocarrier system, since it provides an improved interaction with the biological barriers, namely with the dual blood brain barrier/blood brain tumour barrier, deeming from their small size and electrostatic nature [1,2].

The aim of this work is to develop cNLCs for GBM treatment. [1, 2].Firstly, NLC composition and production were optimized using a Placket Burman factorial design. Secondly, the effect of different cationic surfactants, ranging from serine-based gemini to equivalent conventional synthetic cationic surfactants, on the composition of NLC was assessed. The formulations were evaluated in terms of particle size (PS), polydispersity index (PI) and zeta potential (ZP) and their performance was assessed by *in vitro*cellular studies (cytotoxicity and uptake cellular) using U87 and U373 human cells.

The optimal formulation presented a narrow size distribution (0.224) with a particle size of 43.82± 0.03 nm and ZP of -24±1 mV. The addition of cationic surfactants led to an increased particle size and zeta potential (to positive values), essentially affected by the chain length. Gemini-cNLCs revealed lower cytotoxicity when compared to conventional-cNLCs. A higher uptake was also observed when cationic serine-derived surfactants were included in the formulations.

In conclusion, cNLCs based on serine gemini surfactants are a promising brain drug delivery system for GBM treatment.

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References
[1] H. I. Shah R, Eldridge D, Palombo E, *Composition and Structure. In Lipid Nanoparticles : Production , Characterization and Stability*. 2015.
[2] H. L. Wong, R. Bendayan, A. M. Rauth, Y. Li, and X. Y. Wu, "Chemotherapy with anticancer drugs encapsulated in solid lipid nanoparticles," *Adv. Drug Deliv. Rev.*, vol. 59, no. 6, pp. 491–504, 2007.

Molecular dynamics simulations on glioblastoma: Blood brain barrier mimicry and interactions with chemotherapeutic drugs

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Glioblastoma multiforme (GBM) remainsone of the deadliest cancers worldwide, despite of the current efforts to understand and establish more effective therapeutic approaches. Indeed, the blood-brain barrier (BBB) has been recognized as one of the major obstacles to drug delivery into the brain, thus reducing the efficacy of chemotherapeutic agents in the treatment of GBM patients. [1] Computational models have emerged as a key tool in clinical oncology, being able to simulate and predict several complex tumour phenomena. In particular, molecular dynamics (MD) simulations have been useful to predict the BBB permeability of different compounds and to analyse their behaviouralong the barrier. [2]

In this work, two different lipid model membranes, dipalmitoylphosphatidylcholine (DPPC) and palmitoyloleoylphosphatidylcholine (POPC), were used to mimic the BBB. The two relevant biological molecules under study were temozolomide (TMZ), which represents the current standard of care in GBM patients, and curcumin (CUR), due its antioxidant, antitumor, anti-inflammatory, anti-angiogenic, anti-mitogenic, immunomodulatory, and pro-apoptotic effects. The major purpose was to investigate the interactions between TMZ and CUR in different proportions within hydrated DPPC/POPC bilayer models, which yielded four systems: DPPC (1TMZ:1CUR), POPC (1TMZ:1CUR), DPPC (1TMZ:4CUR) and POPC (1TMZ:4CUR).

The POPC membrane allowed to better mimicking the BBB behavior. CUR was found preferentially in the hydrophobic region of the bilayer, whereas TMZ tended to localize in the hydrophylic region or even outside the bilayer. POPC (1TMZ:4CUR) was considered the system with the most promising results, either due to the membrane behaviour, or by its ability to retain TMZ closer to the hydrophobic region, as desired.

In conclusion, the preferential orientation of compounds within the bilayer were in good agreement with the physicochemical characteristics of TMZ and CUR, as well aswith what is already known about their ability to cross the BBB. This reveals the importance of integrating *in silico* studies in the GBM research, along with *in vitro*/*in vivo* studies, towards better understanding of biological processes.

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References

1. Pourgholi, F., et al., *Nanoparticles: Novel vehicles in treatment of Glioblastoma.* Biomed Pharmacother, 2016. **77**: p. 98-107.
2. Carpenter, T.S., et al., *A method to predict blood-brain barrier permeability of drug-like compounds using molecular dynamics simulations.* Biophys J, 2014. **107**(3): p. 630-41.

Magnetic quaternized chitosan hybrid nanoparticles: potential prospectsfor the uptake of pharmaceuticals from water

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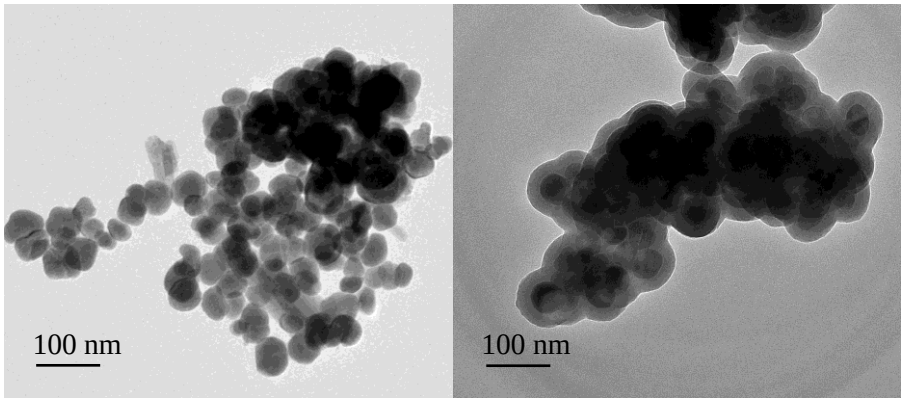
Water pollution caused by pharmaceutical pollutants is one of the most persistent problems on environment all over the world. Due to its potential impact on ecosystems and human health, there is a growing demand to develop new materials for rapid and facile removal of pharmaceuticals from water. To overcome this problem alternative treatment methods are needed. Compared to other methods, adsorption is an attractive process in view of its simplicity of implementation. Among available sorbents, magnetic materials present great practical interest for water treatment because, besides being inexpensive, the pollutants may be removed by the application of an external magnetic gradient. Adequate surface modification of the magnetic particles is required in order to provide high affinity between the magnetic sorbents and the pollutant molecules, and achieve high adsorption capacities.

Keeping these features in mind, the present investigation reports the development of magnetic hybrid nanosorbents based on organic-inorganic coated magnetite (Fe_3O_4) nanoparticles for the uptake of pharmaceuticals from water [1]. The sorbents were prepared using a novel approach for the surface modification of Fe_3O_4 particles with siliceous shells containing a quaternized chitosan polysaccharide. The materials were characterized using electron microscopy, FTIR spectroscopy, elemental analysis and zeta potential measurements. The application of these materials as nano-adsorbents for the efficient removal of emerging chemical pollutants (pharmaceuticals) from water under an external magnetic gradient will be also presented.



TEM images of Fe_3O_4 nanoparticles before (left) and after coated with quaternized chitosan/silica hybrid shells (right).

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References
[1]S.F.Soares, T.R.Simões, M.António, T.Trindade, A.L.Daniel-da-Silva, Chem.Eng.J. 302 (2016) 560–569.

Previous Steps to *in vivo* Studies: Physicochemical and Biological Characterization of a Cationic Gemini Lipid/DOPE-plasmid DNA Lipoplex

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Nucleic acids are used in gene therapy to repair damaged cellular DNA. In this regard, different strategies have been followed: on the one hand, plasmid DNA (pDNA) is used when the introduction of a normal copy of an affected gene can restore healthy cell functioning. However, the necessity of silencing the expression of a certain pathogenic protein leads the use of small interfering RNA (siRNA). Major problems of nucleic acids are their easy degradation by DNAses when are introduced into bloodstream, as well as their negative charge that limits their interaction with the cell membrane. To overcome these barriers, nonviral vectors are used to compact, transport, cross the cellular membrane and delivery the genetic material in a safe way. Cationic lipids (CLs) and, particularly, gemini cationic lipids (GCLs) are raising a remarkable interest by their high effectivity and low toxicity. Their structure, constituted by two cationic heads linked with a spacer, offer a wide variety of potential modifications to improve their biological activity. We have previously reported very promising results of a series of GCLs $(C_{16}Im)_2(C_2H_4O)_nC_2H_4$ (with n = 1, 2 or 3) when transfecting pDNA,[1] and/or silencing activity of siRNA.[2] In both cases, a zwitterionic lipid (DOPE) with pDNA or a neutral lipid (MOG) in the case of siRNA has been used as coadjuvant in the mixed lipid. Following these guidelines, this work is focused on the study of the same series of GCLs with the objective to analyze the behavior of these gene vectors in *in vivo* studies. The lipoplex formed by the mixed lipid $(C_{16}Im)_2(C_2H_4O)_nC_2H_4$/DOPE (n = 3) with a plasmid DNA encoding luciferase (pCMV-Luc) has been characterized by zeta potential to obtain the effective charge. Likewise, agarose gel electrophoresis of the lipoplex against DNAse I, present into human serum, has been carried out. By the other hand, biological *in vitro* studies, the transfection efficiency and cell viability of this lipoplex in several cell lines has been also analyzed. Finally, other preliminary experiments addressed to study the *in vivo* behavior are currently done.

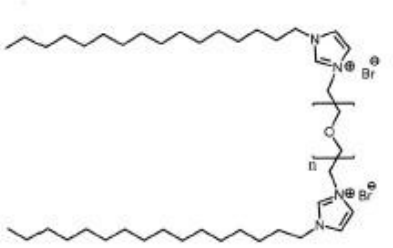

Figure 1. Structure of GCLs series: $(C_{16}Im)_2(C_2H_4O)_nC_2H_4$ (with n = 3)

References

(1) Kumar, K.; Barran-Berdon, A. L.; Datta, S.; Munoz-Ubeda, M.; Aicart-Ramos, C.; Kondaiah, P.; Junquera, E.; Bhattacharya, S.; Aicart, E. *J. Mater. Chem. B* **2015**, *3*, 1495.
(2) Martinez-Negro, M.; Kumar, K.; Barran-Berdon, A. L.; Datta, S.; Kondaiah, P.; Junquera, E.; Bhattacharya, S.; Aicart, E. *ACS Appl. Mater. Interfaces* **2016**, *8*, 22113.

Spectroscopic characterization of biomimetic light harvesting complexes

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Photosynthesis is the process by which plants and bacteria convert light into chemical energy. This process starts with the capture of light by the light harvesting complexes of the plants or bacteria. These complexes are formed by proteins, which contain a few chlorophyll molecules inside [1], or by a protein-independent supramolecular arrangement of hundreds of thousands of chlorophyll molecules, known as chlorosomes in Green Sulphur Bacteria [2]. Once excited, the light harvesting complexes transfer the energy to a reaction center with a nearly perfect quantum efficiency, higher than that calculated for the classical mechanism of Foster Resonance Energy Transfer. Two-dimensional electron spectroscopy techniques have demonstrated in recent years that this high efficiency is due to a quantum coherence energy transfer [3]. Here, we propose the development of simple biomimetic light harvesting complexes, a self-assembly of chlorophyll molecules, inspired in chlorosomes, as models for spectroscopic studies of this quantum phenomenon. These studies may help us understand the complexity of the photosynthetic process, which may help develop new technologies in the renewable energy field.

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References
[1] Liu, Z., Yan, H., Wang, K., et al. (2004). *Nature*, 428(6980), 287-292.
[2] Oostergetel, G. T., van Amerongen, H., & Boekema, E. J. (2010). *Photosynthesis research*, 104(2-3), 245-255.
[3] Panitchayangkoon, G., Hayes, D., Fransted, K. A., et al. (2010). *Proceedings of the National Academy of Sciences*, 107(29), 12766-12770.

Catanionic Vesicles Composed of Threonine-based Surfactants: Phase Behavior and Microstructure

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Catanionic vesicles built up from conventional surfactants have been extensively studied not just from a fundamental physicochemical point of view, but also in the perspective of practical considerations, such as templating nanomaterials, gelation, rheological control, and drug and gene delivery [1]. From a pharmaceutical and biomedical point of view, catanionic systems formed by amino acid-based surfactants present higher levels of biocompatibility and biodegradability, with good interfacial performance and multifaceted self-assembly, from elongated micelles to vesicles, liquid crystalline nanoparticles and other supramolecular aggregates [2,3]. In this work, our aims were to synthesize pH-sensitive single-chained surfactants derived from the amino acid threonine and to explore their vesicle-forming ability. The compounds have simple monomeric configuration and different alkyl chain length, and are designated by *n*ThrNa, where *n* is the number of carbon atoms in the hydrocarbon chain, ranging from 8 to 16 (see figure). After *cmc* determination and characterization of the surface properties of the neat threonine surfactants, the most suitable threonine amphiphiles were used in catanionic mixtures. Phase behavior studies and microstructural characterization of several aqueous mixtures based on 12ThrNa as the anionic surfactant, and in gemini serine-based and gemini conventional surfactants as the cationic surfactants. Detailed results from polarized light microscopy, cryogenic scanning electron microscopy (cryo-SEM), dynamic light scattering (DLS) and zeta potential measurements will be presented and discussed.

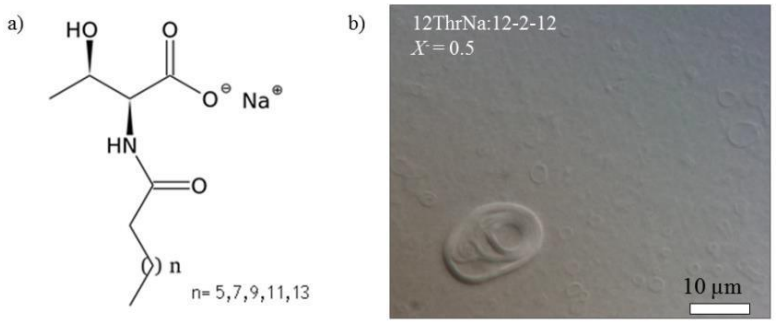

Figure. (a) General molecular structure for the novel threonine-based surfactants; (b) micrograph of vesicles dispersion obtained by polarizing light microscopy from the 12ThrNa:12-2-12 systems, at X_{-} =0.5.

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References
[1] Marques E.F., Surfactant Vesicles: Formation, Properties and Stability, in Encyclopedia of Surface and Colloid Science, Taylor & Francis, New York, 2010, 1:1, 1-20.
[2] S.G. Silva, M.L do Vale and E.F. Marques, Chem. Eur. J., 21 (2015) 4092-4101.
[3] S.G. Silva, I.S. Oliveira, M.L. do Vale and E.F. Marques, Soft Matter, 10 (2014) 9352-9361.

Magnetite-supported gold nanostars for SERS detection of antibiotics

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The presence of antibiotics in effluents has been considered a global environmental problem due to bioaccumulation in aquatic life before entering into drinking water sources. Particularly, the occurrence of these pharmaceutics in aquatic ecosystems contributes to the increasing resistance of some pathogenic microorganisms to conventional antibiotics [1]. The vestigial detection of such antibiotics is extremely important, however most conventional methods for detection of antibiotics are time and cost consuming. In this context, sensitive procedures for detecting vestigial antibiotics are of great relevance for water quality monitoring and therefore to guarantee its sustainable supply. Our interest in this field, prompted us to develop new analytical platforms for surface-enhanced Raman scattering (SERS) detection of bioanalytes dissolved in water [2,3].
As such, we herein report the seed-mediated growth of colloidal magnetite-supported gold nanostar (Mag-AuNS) particles. These nanomaterials were then investigated as active SERS materials for the detection of tetracycline (TC) in aqueous solution. Such multifunctional combine magnetic and plasmonic components whose preparation involved the *in situ* synthesis of Au NS supported on ferromagnetic nanoparticles, with no need of surfactant or polymer stabilizers [4]. The ability of such hybrid materials to act as SERS platforms for the detection of TC was systematically evaluated in a range of operational conditions. Additionally, microscopic methods, including Raman confocal microscopy, have been employed to characterize the as prepared SERS substrates and to monitor the sensing process.
Taking advantage of the magnetic properties of the nanocomposite, adsorption studies were carried out for simultaneous use in water purification and detection of vestigial amounts of antibiotics. These results will be discussed on a perspective of potential use of these materials for laboratory monitoring and water treatment units.

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References
[1] C. Xi, Y. Zhang, C. F. Marrs, Appl. Environ. Microbiol., 75 (2009) 5714–5718.
[2] P. C. Pinheiro, S. Fateixa, H. I.S. Nogueira and T. Trindade, Spectrochim. Acta A, 101 (2013) 36−39.
[3] P. C. Pinheiro, S. Fateixa, H. I. S. Nogueira and T. Trindade, J. Raman Spectrosc., 46 (2015) 30-50.
[4] Y. Wang, L. Polavarapu and L. M. Liz-Marzán, ACS Appl. Mater. Interfaces, 6 (2014) 21798−21805.

Photothermal conversion efficiency and cytotoxic effect of gold nanorods stabilized with chitosan, and overcoated with alginate or PVA

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Gold nanorods (GNR) use has been proposed in medical applications because of their intrinsic photothermal properties. However, the presence of CTAB molecules adsorbed onto the surface of GNRs results in a highly cytotoxic GNR system. In this work we replace the CTAB molecules with a thiolated chitosan. Once chitosan coated GNRs (Chi-SH-GNR) were attained, a film of alginate (Alg-Chi-SH-GNR) or polyvinyl alcohol (PVA-Chi- SH-GNR) was deposited onto the surface of Chi-GNR by a layer-by-layer process. The photothermal conversión efficiency for the GNR systems was determined irradiating the GNRs suspended in aqua media with a CW 808 nm diode laser (CNI, China). The cytotoxicity effect and the photothermal cellular damage of GNR systems were evaluated on a breast cancer cell line. Results show that polymer coats did not affect the transduction photothermal efficiency. Values around 50% were obtained for the different coated gold nanorods. The cytotoxicity of coated gold nanorods diminished significantly compared with those GNR stabilized with CTAB. The laser irradiation of cells treated with gold nanorods showed a decrease in their viability compared with the cells treated but no irradiated.

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References

[1] D.K. Roper, W. Ahn, M. Hoepfner, Microscale heat transfer transduced by surface plasmon resonant gold nanoparticles, J. Phys. Chem. C 111 (2007) 3636–3641.
[2] K.S. Lee,M.A. El-Sayed, Dependence of the enhanced optical scattering efficiency relative to that of absorption for gold metal nanorods on aspect ratio, size, end-cap shape, and medium refractive index, J. Phys. Chem. B 109 (2005) 20331–20338.

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