MultiComp

Aveiro Spring Meeting 2019

Book of Abstracts

University of Aveiro
21st – 22nd March, 2019

COST Action CA15107
MULTICOMP
MULTI-FUNCTIONAL NANO-CARBON COMPOSITE MATERIALS NETWORK

Aveiro Spring Meeting
March 21st – 22nd, 2019
Aveiro, Portugal

Organized by
CICECO – Aveiro Institute of Materials
University of Aveiro

Foreword

Dear Colleagues and Meeting Participants

We are pleased to welcome you to the **MULTICOMP Aveiro Spring Meeting 2019** taking place at University of Aveiro, Portugal, from 21st to 22nd March 2019.

The meeting aims to share information on the emerging field of nano-carbon material composites, including (1) the adequate dispersion of the nano-carbon reinforcement material, and (2) the development of strong enough interfacial bonding between the nano-carbon reinforcement elements and the composite matrix. As MULTICOMP (MULTI-FUNCTIONAL NANO-CARBON COMPOSITE MATERIALS NETWORK) COST Action CA15107 aims to bring together theorists, experimentalists and industrialists in the field of nano-carbon materials technology, the Aveiro Spring Meeting 2019 is especially thought to promote mutual collaborations and define common strategies among the MULTICOMP partners, as well as attract additional scientists and companies into the Action.

During the two meeting days, we will have 3 Keynotes, 28 oral presentations, and 52 posters.

We hope, this meeting will be an excellent forum to hold scientific discussions in a relaxed atmosphere, and to exchange experiences, enriching ourselves. It will also contribute to strengthen scientific collaborations between us, seeding new joint activities. For the younger scientists, in particular, it will be a great opportunity to network with other fresh and seasoned researchers.

The attractive city of Aveiro offers cultural experiences and entertainment possibilities that will enrich and complement the meeting. The social programme will include the degustation of Aveiro’s traditional sweet “ovos moles” and Porto wine during a trip on board of the typical Moliceiro boat through the channels of the Ria de Aveiro, finishing with the conference banquet at Fábrica de Cerâmica Jerónimo Pereira Campos, an old ceramics factory.

We warmly welcome you to Aveiro. We very much hope that you will enjoy and profit from the meeting, encounter new and old colleagues, and take some time to visit our beautiful home town and perhaps its deep blue surroundings.

Local Organizing Committee

Cláudia Nunes

Helena Oliveira

Paula Ferreira

Committees:

Conference chairs:

Helena Oliveira (University of Aveiro, CICECO & CESAM, Department of Biology)

Paula Ferreira (University of Aveiro, CICECO – Aveiro, Department of Materials and Ceramics Engineering)

Sharali Malik (Karlsruhe Institute of Technology (KIT), Institute of Nanotechology (INT))

Local organizing:

Cláudia Nunes (University of Aveiro, CICECO, Department of Chemistry)

Helena Oliveira (University of Aveiro, CICECO & CESAM, Department of Biology)

Paula Ferreira (University of Aveiro, CICECO – Aveiro, Department of Materials and Ceramics Engineering)

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Scientific Programme

Thursday, March 21st

08h45-09h00	**Registration**
09h00-09h10	**Welcome**
09h10-09h55	**Invited Keynote Talk I - Session Chair Fil Ruddock**
	Paula A. A. P. Marques *Perspectives of graphene-based composites: Significant features and applications.*
09h55-10h40	**FLASH Presentations (6 x 5 min talks)**
	Raul Arenal *Advanced TEM Studies on Nanodiamonds*
	Christa Schimpel *A Potential Approach to Assess and Control the Potential Risks Related to Graphene Nanoplatelets*
	Ivana Capan *Electrically active defects in semiconductors*
	Anthony Blue Carter *MultiComp Research Dissemination: Research Gate and More*
	Polona UMEK *The role of water in the transformation of protonated titanate nanoribbons to anatase nanoribbons*
	Carla Bittencourt *Hydrophilicity and carbon length chain effect on gas sensing mechanism for thiol SAM/CNT sensor*
10h40-11h20	**Coffee Break and Posters**
11h30-12h15	**Invited Keynote Talk II – Session Chair Silvia Marchesan**
	Daniel Ugarte *Study of structural distortions in individual nanostructures by spatially resolved precession electron diffraction (SPED)*
12h15-13h00	**FLASH Presentations (6 x 5 min talks)**
	Michal Bodik *The alignment of carbon nanotubes on a water surface*
	Radmila Tomovska *UV Protective Waterborne Polymer Coatings Based on Hybrid Graphene/Carbon Nanotube Radicals Scavenging Filler*
	Aleksandra Miletić *Carbon-filler loaded cellulose nanofiber-based membranes for waste water treatment*
	Hilal Demir Kıvrak *Synthesis of doped Graphene by CVD technique, characterization, and investigation of their glucose sensor sensitivities*
	Rachel McLaren *Development of New Graphene-Based Materials Containing Poly-yne Groups, For Advanced Applications*
	Ieva Kranauskaite *Electrical properties of onion-like carbon composites*
13h00-14h30	**Lunch Break** – Opportunity to Network

14h30-15h15	**Invited Keynote talk III – Session Chair Serkan Unal**
	Alexandra Fabricius *An Introduction to Standardization – How can it help to promote innovations?*
15h15-16h00	**FLASH Presentations (6 x 5 min talks)**
	Lucas Luciano Cullari *Nanoplatelets Enhancement of Water Barrier Properties in Polymer Nanocomposties*
	Silvia Giordani *Carbon Nano-Onions*
	Antonio J. Paleo *Hybrid solid-state supercapacitors based on AC/MnO2 cotton fabric electrodes*
	Valentina Gargiulo *From raw to added value materials: production of carbon-based materials for gas adsorption applications as possible route for biomass valorization*
	Chris Ewels *Novel nanocarbon design from first principles modelling and organic synthesis*
	Jacek Wychowaniec *Elastic flow instabilities and macroscopic textures in graphene oxide lyotropic liquid crystals*
16h00-17h00	**Beverage break and Posters**
17h00-18h30	**FLASH Presentations (10 x 5 min talks) – Session Chair Ioannis Remediakis**
	Polina Kuzhir *Electromagnetic express non-invasive test of chloroprene rubber after long-term ultraviolet, oil immersion and thermal degradation*
	Ivan Ristic *Synthesis of hybrid biobased conductive materials*
	Daphne Davelou *Edge states in graphene and graphene-like materials*
	Fiodor Braniste- *Hybrid multifunctional nanostructures based on Aerographite and semiconductor materials*
	Branislav Stankovic *Application of fractal kinetics on non-isothermal dehydration of fullerol*
	Liutauras Marcinauskas *Synthesis of doped amorphous carbon films by magnetron sputtering*
	David Tomeček *A photoregenerative method for low temperature NO2 sensors*
	Marta d'Amora *Comparative toxicity of carbon nanomaterials on zebrafish*
	Maria Kanidi *Films of polymer blends with tunable wettability on flat and microstructured silicon surfaces*
	Ana Barra *Synthesis and characterization of electrical conductive biocomposites from natural precursors*
19h00-20h00	**Sunset with *Porto* wine and *Ovos Moles***
20h00-23h00	**Conference Dinner**

Posters

1. **Oren Regev** - Stronger Cement
2. **Juras Banys** - Dielectric relaxation in PDMS/TiO2 nanocomposites
3. **Monika Wysocka-Zolopa** - Synthesis, morphology and electrochemical properties of polypyrrole nanoparticles doped with fullerene C60
4. **Mariana R. F. Silva** - The benefit of carbon nanostructures addition to titanium oxide for benzene photocatalytic degradation in air
5. **Maria Rybarczyk** - Hard carbon materials and their application as an anode in sodium-ion batteries
6. **Filip Marinkovic** - The influence of weight fraction of reduced graphene oxide on thermo-physical properties of poly(MMA/BA/HEMA) latex composites
7. **Jelena Jovanovic** - The effects of reaction conditions on the physico-chemical and morphological properties of reduced graphen-oxide – gelatin nanocomposite hydrogels
8. **Aleksandras Iljinas** - Formation of amorphous carbon films using Ar-C2H2 and Ar-C2H2-H2 plasma
9. **Ana Teresa Brandão** - Deep eutectic solvent/carbon materials interfacial studies for potential energy storage applications – Effect of carbon modification
10. **Mark Eaton** - Controlling Microstructure in Nanocomposites using Magnetic Fields
11. **Claudio Larosa** - Graphene flakes dispersed in polycarbonate: thin films composites and optical properties
12. **Uwe Popp** - Surface effects of sintered steel processed by material extrusion
13. **Roberto Di Capua** - Spectroscopic study on Eumelanin / Graphene-like hybrids by nuclear magnetic resonance and photoemission spectroscopy
14. **Karol Strutynski** - Electronic structure of Two-Dimensional Conjugated Microporous Polymers
15. **Juan P. Fernandez-Blazquez** - Effect of Graphene Nanoplatelets in the dynamic crystallization of PEEK
16. **Miroslav Huskić** - Effect of morphological structure on physical properties of SWCNT/PE nanocomposites
17. **Malamatenia Koklioti** - Photodegradation of RhB by functionalized MoS2 sheets and core-shell Ag@Au nanoclusters
18. **Malamatenia Koklioti** - Pd@M (M=Ni, Cu, Co) nanoparticles / graphene ensembles toward the oxygen electroreduction
19. **Ricardo M. F. Fernandes** - Adsorption, Kinetics, and Bundle Size Distribution as Determining Factors in Surfactant-Assisted Dispersions of Carbon Nanotubes
20. **Bárbara Abreu** - Comparing the dispersibility of carbon nanotubes and graphene using amphiphilic molecules: similarities, differences and trends
21. **Eduardo Marques** - Gemini surfactants as efficient dispersants of multiwalled carbon nanotubes
22. **Mirtha A. O. Lourenço** - Tuning carbon nano onions for CO2 capture
23. **Jorge Diogo Marques Laranjeira** - DFT investigations of 3D C60 polymers with ordered binary-alloy type structures
24. **Andreia F. Sousa** - Roots towards innovation in sustainable poly(2,5-furandicarboxylate)s polymeric materials

25. **Gagik Shmavonyan** - The Nano-patterning of Two-dimensional Atomic Structures by Focused Ion Beam Treatment
26. **Fábio Campos** - Pulmonary toxicity of inhaled graphene-based nanoplatelets
27. **Anastasios Stergiou** - Regioselective Synthesis of an Equatorialface Bisadduct of Azafullerene. Molecular manipulation towards efficient fullerene-based electron acceptors.
28. **Abdülkadir Sezai SARAC** - Polyacrylonitrile Based Stabilized Nanofibers and Carbon Nanofibers
29. **Ivan Brnardić** - Characterisation of nanocomposites based on Al-alloy and multiwall carbon nanotubes prepared by industrial High Pressure Die Casting method
30. **Matej Micusik** - Electrospinning of ethylene vinyl acetate/ multiwall carbon nanotubes fibers
31. **Juras Banys** - Synergy effects in ferroelectric polymeric composites
32. **Zélia Ribeiro Alves** - Zinc oxide – reduced graphene oxide nanocomposite dispersed in sepiolite to enhance alginate film properties
33. **Ivan Radović** - Wake potential in a graphene-sapphire-graphene structure
34. **Jonathan Nitschke** - Complex supramolecular systems via subcomponent self-assembly
35. **Michela Alfè** - Easy tools for microtexture nanoparticles tuning: exploring the flexibility of a spark generator system
36. **Irina Kuehne** - Surface attachment of Mn(III) SCO compound on few-layer graphene
37. **Jadranka Blazhevska Gilev** - Doping of the graphene with Pt nanoparticles by pulsed laser deposition
38. **Manuela Meloni**- Controlled Assembly of Graphene Networks Using Polymer Latex Crystal Templates
39. **Evgeni Ivanov** - PLA-based multi-functional nanocomposites with improved properties for FDM 3D printing
40. **Aleksandra Ivanoska-Dacikj**- Biodegradable, elastic, electrospun polyurethane/graphene oxide scaffolds for soft tissue engineering application
41. **Amra Bratovcic** - Carbon nanomaterials in removing of organic compounds from water
42. **Tony D. Keene** Towards Graphite- and Graphene-supported Heterogeneous Ullmann Catalyst Composites
43. **Eduardo Ruiz-Hitzky** - Carbon-clay nanostructured materials: application in the catalytical hydrodechlorination of chlorophenols
44. **Istvan Furo** - Polymer/nanotube composites: insights from NMR studies
45. **Valentina Veselinović** - Mechanical properties of newly formed nanomodified PMMA/AuNPs denture base material
46. **Olga Karavai** - Graphene-coated textiles: a platform for wearable electronics
47. **Olena Okhay** - Freestanding electrodes based on reduced graphene oxide
48. **Fatima Z. Bouanis**- Functionnalized CNTFETs for gas sensing
49. **Fatima Z. Bouanis** - Graphene nanoplatelets coating for corrosion protection of aluminum substrate
50. **Tamás Szabó** - Ultrafine Dispersion of Graphene Oxide Nanoplatelets in a Magnetic Iron Oxide Matrix by Heterocoagulation
51. **Sónia Fraga** - Cyto- and genotoxicity of different classes of manufactured nanomaterials in alveolar epithelial cells
52. **Philippe Poulin** - Soft graphene nanocomposites for mechanical sensing and energy harvesting applications

Friday, March 22nd

09h30-10h30	**MC Meeting**
10h30-10h50	Coffee Break
10h50-13h00	**MC Meeting concluded**
13h00-14h30	Lunch Break
14h30-16h00	**WGs Meetings**
16h00-18h30	Networking

Index

Abstracts

KN1 - Perspectives of graphene-based composites: Significant features and applications.

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During the past few years, graphene and its based materials (GBM) have outstandingly emerged as key nanomaterials for boosting the performance of commercial, industrial and scientific related technologies. The popularity of these novel nanomaterials, for example in biomedical and environmental engineering, is due to its excellent biological, electronic, optical and thermal properties that, as a whole, surpass the features of commonly used nanomaterials and consequently open a wide range of applications so far within the reach of science fiction. In this talk, the potential of GBM, particularly graphene oxide (GO), in the expanding biomedical and environmental fields will be highlighted. References to different preparation methodologies of GO containing composites from two dimensional to three dimensional structures will be presented. Also, some of the major challenges related to the synthesis and safety of GBM will be briefly discussed because of their critical importance in bringing this class of carbon materials closer to the real applications.

Acknowledgement
CENTRO-01-0145-FEDER-030513, PTDC/NAN-MAT/30513/2017 and UID/EMS/00481/2019

KN2 - Study of individual nanosystems by electron microscopy: in-situ experiments and advanced characterization methods.

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The new physical and chemical properties of nanosystems place them as one of the most promising element to develop new technologies. However, the detailed assessment of atomic structure and chemical modifications in nanomaterials still represents a challenge, rendering difficult the development of basic understanding and technological use. We will discuss the application of electron microscopy techniques to analyze in detail the structural and electronic properties of individual nanostructures. The atomistic aspects associated with sample modification can be at present easily followed by real-time in situ atomic resolution transmission electron microscopy. The detailed analysis of different nanostructures by advanced electron microscopy methods will be discussed, including carbon onion or carbon nanotubes, noble metal nm-wide rods and semiconductor nanowires.

KN3 - An Introduction to Standardization – How can it help to promote innovations?

Alexandra Fabricius,
DKE German Commission for Electrical, Electronic & Information Technologies of DIN and VDE

Standards are part of everyday life. They ensure product safety and compatibility, provide consumer confidence, decrease trade barriers and enable collaboration. The International Standards Developing Organizations IEC and ISO involve all stakeholders in an open and transparent process to assure the resulting standard is widely accepted. Standards are subject to regular maintenance to make sure they represent the current “state of the art” of a technology.

Standards are useful in well-established areas. However, standardization can also help new technologies to succeed in the market, e.g. through creating an accepted framework or providing agreed terminology and thus enabling communication across domains.

This presentation will give a brief introduction of standards and the standardization process in IEC. It will inform why standardization is important for innovative technology fields and will provide an overview of the activities in the field of nanotechnologies as an example for an emerging technology.

F01 - Advanced TEM Studies on Nanodiamonds

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[b] *Fundacion ARAID, 50018 Zaragoza – Spain*

Chemical analyses at the local (sub-nanometer/atomic) scale are crucial for improving the understanding of materials. For instance, for doped carbon nanostructures (as those of diamond family), these analyses are critical because their properties strongly depend on the chemical environment/configuration of the dopants [1-4]. Electron energy-loss spectroscopy (EELS), developed in an aberration-corrected TEM (having access to a close to 1 angstrom electron probe), is an essential and powerful technique to perform such local chemical analyses [2-4].

In this contribution, we will present a detailed study of the structure and local composition of nitrogen-doped ultrananocrystalline diamond (UNCD) films [5-8]. Under normal process conditions, these UNCD films are highly electrically insulating, but they can become highly conducting when Ar is substituted in the synthesis gas with some of N2 [1, 4-8]. The formation of these NWs starts to appear when the N2 content in the gas phase reaches about 10% in volume. From these studies, we concluded that the insulator-metal transition of these films is strongly correlated with the formation of these diamond NWs. Indeed, these NWs are enveloped by a sp2-based carbon layer providing the conductive path for electrons [5-8].

In summary, these studies elucidate crucial questions concerning the local composition (atomic configuration) of these materials. This detailed knowledge is essential for better understanding the outstanding properties of such materials.

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[3] P. Ayala, R. Arenal, A. Rubio, A. Loiseau, T. Pichler, Rev. Mod. Phys. 82, 1843 (2010).
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[8] R. Arenal, F. Hage, Q. Ramasse, D.M. Gruen, to be submitted.

Acknowledgement
[*] This work was supported by the Spanish MINECO (MAT2016-70776-P), the EU H2020 program Marie Sklodowska-Curie EnEx (Grant Agreement 642742), the EU H2020 & APCIN-MICINN Spain (JTC-2017 Flag-ERA GATES project) and the EU H2020 program "Graphene Flagship" (Grant Agreement 785219).

F02 - A Potential Approach to Assess and Control the Potential Risks Related to Graphene Nanoplatelets

C. Schimpel[1], S. Resch[1] and A. Falk[1]
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Efforts are currently being made to integrate the Safe-by-Design (SbD) approach into the development of new nanomaterials and their application. In this work we present a case study related to the up-scaling of graphene manufacturing (patent WO 2016/042305 A1) and graphene-based ink formulations. This study was carried out within the framework of an EU funded project called INSPIRED (Grant Agreement No 646155) [1] which aims to demonstrate the high throughput synthesis and scale-up of nanomaterials for printed electronic applications. Our approach [2] is addressed to eliminate exposures and minimize risks that may be related to the manufacturing processes, introducing the SbD concept in the design/innovation and development phases of the pilot plant. It includes the identification of potential exposure scenarios, the use of qualitative and semi-quantitative tools to prioritize them (ISO-CB 12901, Stoffenmanager Nano, ECETOC TRA) and the measurement of occupational exposure, both at lab and pilot scale. Occupational exposure monitoring is performed following the OECD harmonized tiered approach.

Due to latest findings occupational release/risk is not expected since tasks are performed under safeguarded conditions (e.g., risk is controlled using appropriate safety measures like LEV, PPE, waste management measures). Results from the exposure monitoring at lab scale from previous works indicated no graphene release into the workplace environment. In addition, exposure assessment of the pilot plant (including up-scaled processes for bulk production of graphene and ink formulation) was performed, following NIOSH methods based on filter sample collection and posterior mass concentration determination and SEM/EDX analysis. The results from the analysis of the samples collected revealed that worker exposure to GNPs was low, below the selected limits (in mass concentration), confirming that control measures were appropriate.

In conclusion, the SbD approach can be easily implemented the innovation process and thus represents a suitable concept to manage uncertainties/potential risks and thus lowering the commercialization barrier for innovative nanotechnology driven products based on graphene.

References
[1] http://www.nano-inspired.eu/
[2] Schimpel, Christa, et al. "A methodology on how to create a real-life relevant risk profile for a given nanomaterial." Journal of Chemical Health and Safety 25.1 (2018): 12-23.

F03 - Electrically Active Defects in Semiconductors

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Electrically active defects in semiconductors introduce energy levels into the energy band gap. Those levels act as traps for carriers, and therefore strongly affect the properties of semiconductor devices. Deep level transient spectroscopy (DLTS) is an experimental tool for studying electrically active defects in semiconductors. DLTS establishes fundamental defect parameters and measures their concentration in the material. Some of the parameters are considered as “defect fingerprints" used for their identifications and analysis. There is an extension to DLTS known as a high-resolution Laplace DLTS (Laplace-DLTS). Laplace-DLTS is an isothermal technique in which the capacitance transients are digitized and averaged at a fixed temperature. Then the defect emission rates are obtained with a use of numerical methods being equivalent to the inverse Laplace transformation. The main advantage of Laplace DLTS in comparison to conventional DLTS is the increase in energy resolution. We shall present results of DLTS and Laplace-DLTS study of electrically active defects in 4H-SiC material.

Acknowledgement

This work is financially supported by the NATO SPS Programme, under project no. 985215.

References

[1] Ivana Capan, Tomislav Brodar, Takeshi Ohshima, Shin-ichiro Sato, Takahiro Makino, Željko Pastuović, Rainer Siegele, Luka Snoj, Vladimir Radulović, José Coutinho, Vitor J. B. Torres, Kamel Demmouche, Double negatively charged carbon vacancy at the h- and k- sites in 4H-SiC: Combined Laplace-DLTS and DFT study, Journal of Applied Physics 123 (2018) 161597.

[2] Ivana Capan, Tomislav Brodar, Jose Coutinho, Takeshi Ohshima, Vladimir Markevich, Anthony Peaker, Acceptor levels of the carbon vacancy in 4H-SiC: combining Laplace deep level transient spectroscopy with density functional modeling, Journal of Applied Physics 124 (2018) 245701.

F04 - MultiComp Research Dissemination: Research Gate and More

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> ‘Research is of no use unless it gets to the people who need to use it’
> - Professor Chris Whitty Chief Scientific Adviser for DHSC

Dissemination broadly refers to the transfer of research-based knowledge, it is now recognised as a vital component of an academic’s job and provides a foundation for collaboration and future projects. Moreover, it is increasingly important to communicate results to the general public who provide the funding for many research studies through their taxes. In recent years many funding scheme applications have an additional section requiring researchers to demonstrate how they have considered dissemination. Dissemination is a broad process which can take many forms, most of which are a common occurrence and range from formal academic publications and conference attendance to quick emails with potential colleagues. In the case of MultiComp, dissemination refers to sharing our research findings with both the scientifically literate and a general audience, this should include modern technology to reach a wider audience. Members of MultiComp are already doing this using YouTube videos and a planned video series, however there are further opportunities that all members can participate in such as Research Gate and Twitter.

Many companies and universities have discovered that bad dissemination can harm a brand or project further than no dissemination. My talk will address “good” and “bad” dissemination techniques, the use of research gate and twitter to publicise research, and hopefully provide the basis for discussion on the best ways for us to increase the research impact of MultiComp funded work and activities.

#MultiComp #Chemistry #Graphene #Research #Abstract #Presentation

F05 - The role of water in the transformation of protonated titanate nanoribbons to anatase nanoribbons

Melita Sluban and Polona Umek
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Titanium dioxide has been a subject in extensive research over the last decades due to the material's photoactivity. Since one-dimensional morphology is beneficial than/over the zero-dimensional one when considering charge separation, charge transfer and a defect amount present in material, 1D protonated titanates are appealing TiO_2 precursors.

The transformation from protonated titanate to TiO_2-B and anatase has already been a subject of intense research. The transformation is a condensation as presented with the equation $H_2Ti_3O_7 \rightarrow 3\ TiO_2 + H_2O$. Theoretically, condensations can be achieved either with (i) enough large energy input to overcome the activation energy of the reaction, or (ii) with lowering the activation energy, that is catalysis where typical catalysts for condensations are acids and bases. In practice, the first way is performed with calcination of protonated titanate in air or some other atmosphere whereas the catalysis is performed in aqueous media under hydrothermal or even ambient conditions. Despite several investigations, some questions have still remained: How does protonated titanate behave under basic hydrothermal conditions and how do different bases influence the transformation? In addition, what is the exact role of water or other liquid reaction media?

In this work the investigation of the transformation of protonated titanate nanoribbons to TiO_2 was motivated with three goals: (i) to understand the behavior of HTiNRs under hydrothermal conditions over the whole pH range, (ii) to determine the role of water in the transformation, and (iii) to explain the product morphology in regard to reaction environment. Therefore, the transformation reactions of HTiNRs were conducted under various hydrothermal and solvothermal conditions as well as with annealing in static air. A deeper insight into the transformation process as well as the product formation was additionally ensured with Zeta potential measurements and a detailed electronic microscopy coupled with crystallography.

F06 - Hydrophilicity and carbon length chain effect on gas sensing mechanism for thiol SAM/CNT sensor

Juan Casanova-Cháfer[1], Carla Bittencourt[2*], Eduard Llobet[1]
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[2]Chimie des Interactions Plasma-Surface (ChIPS), Research Institute for Materials Science and Engineering, Université de Mons, Avenue Copernic 1, Mons, Belgium

Self-Assembled Monolayers (SAMs) attached to decorated Multi-Wall Carbon Nanotubes (MWCNTs) with gold nanoparticles sensors were designed to study the effect of carbon length chain and hydrophobicity of thiol functional group on gas sensing response. In this work it was measured polar gases, such as NO_2 and ethanol, to analyze the chemoresistive response. In addition, the gas sensing behavior was studied under moisture conditions. Possible gas sensing mechanisms were proposed to explain the effect of different SAMs on the sensor response. The present report can promote the research toward the fabrication of more selective gas sensors for monitoring specific toxic gases

Acknowledgement
J. Casanova-Cháfer is supported by a Martí i Franquès pre-doctoral fellowship from Universitat Rovira i Virgili (URV), and E. Llobet is supported by the Catalan Institution for Research and Advanced Studies via the ICREA Academia Award. CB is a Research Associate of the National Funds for Scientific Research (FRS-FNRS, Belgium). We all thanks The COST Action CA15107 (MultiComp).

F07 - The alignment of carbon nanotubes on a water surface

Bodik, M., Maxian, O.*, Hagara, J., Siffalovic, P., Jergel, M. and Majkova, E
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The oriented self-assembled films of single-walled carbon nanotubes (SWCNTs) over large areas can play an important role in future applications. We tracked the orientation of SWCNTs in Langmuir film in real time by means of *in-situ* polarized Raman microscopy.

Experimentally, we observed a gradual shift of orientation of SWCNTs towards fully oriented film as a function of surface pressure. In order to elucidate the orientation of SWCNTs in Langmuir films, we performed numerical simulations. The experimental findings are in good agreement with our numerical simulations.

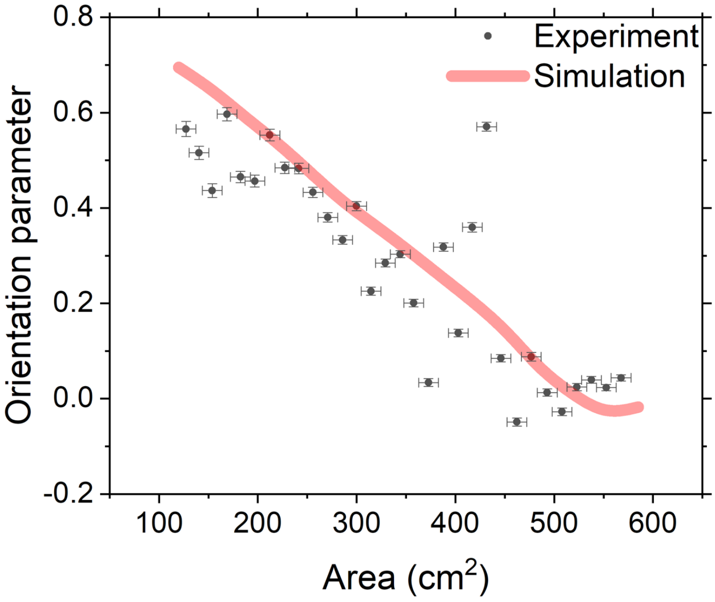

Fig. 1: Orientation parameter of SWCNTs obtained from the experiment (black squares) and simulation (red curve). The orientation parameter is equal to 1 and 0 for perfect and random orientation, respectively.

Acknowledgement
COST Association and COST Action CA15107 Multi - Functional Nano - Carbon Composite Materials Network (MultiComp) is acknowledged for the financial support.

References

[1] - CAO, Qing, et al. Arrays of single-walled carbon nanotubes with full surface coverage for high-performance electronics. Nature nanotechnology, 2013, 8.3: 180.

F08 - UV Protective Waterborne Polymer Coatings Based on Hybrid Graphene/Carbon Nanotube Radicals Scavenging Filler

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UV degradation is one of the most important challenges of waterborne coatings in exterior applications, which ones solved, may decrease significantly the maintaining costs and extend the lifetime of our infrastructures, equipment and vehicles. Addition of radical scavenging species within the polymer matrix is one of the ways to address this issue [1]. In this work, hybrids of graphene (G) and multiwall carbon nanotubes (CNT) in different ratios were used as radical scavenging species. Advantage was taken of the facilitated charge transfer between both G and CNTs that was expected to improve the capture and resonant stabilization of the captured radicals [2,3]. Evaluated by EPR spectroscopy, it was found that the hybrid made of G/CNTs in ratio of 10:1 efficiently captured and quenched the free radicals. The waterborne polymer composites containing 1 wt% of hybrid G/CNT were synthesized by in situ miniemulsion free radical polymerization. As heterogeneous reaction, it offers opportunity to have physically separated the radical initiator (in organic phase) and the radical scavenging filler (in water phase). The resulting polymer composites, beside excellent mechanical resistance, presented exceptional stability under accelerated aging conditions during 400h, suppressing almost completely the UV photodegradation. This performance was attributed to the efficient radical scavenging of the G/CNTs hybrid filler distributed within polymer matrix

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F09 - Carbon-filler loaded cellulose nanofiber-based membranes for waste water treatment

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Waste water from textile dyeing is big environmental problem because it contains organic dyes which cause serious problems to animal species in water flows. Many different techniques and approaches are developed for water treatment and removal of organic compounds and many of them are based on absorption using different active substrates.

Carbon nanofillers can be successfully used for removal of gases, organic and inorganic ions and substances, heavy metals and other toxic materials [1].

In this work, nanofiber-based membranes were prepared from cellulose-based solutions using 4 different carbon fillers: exfoliated graphene, modified MWCNT, unmodified MWCNT and bioactive carbon in three concentrations 0.5, 1 and 2 wt%. Non-wovens prepared this way are used for removal of organic dye from water and ability of absorption and number of cycles until saturation were examined. Morphology and mechanical properties were also examined.

Acknowledgement: Authors would like to thank COST Action MultiComp CA 15107, and Ministry of Education, Science and Technological Development Republic of Serbia for funding project III45022.

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F10 - Synthesis of doped Graphene by CVD technique, characterization, and investigation of their glucose sensor sensitivities

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Enyzme based electrodes were usually employed for the preparation of electrochemical sensors. Electrochemical oxidation (or reduction) of these molecules consists of many process including adsorption, electron transport, and consecutive chemical reactions. In recent years, it is possible to direct oxidation or recution of these molecules on solid electrode surface by the synthesis of new nanomaterials and the application of these materials as modified electrode material. For these non-enzymatic sensors, the size of nanocrystals affects the sensor activity and sensitivity. Thus, the adjustment of the particle size and the arrangement of the surface electronic way to increase sensor activity requires nano-engineering experience. The depositon of the metal atoms on the graphene sheets has important effects on the graphene properties. graphene / graphene oxide modified via metal or metal oxide nanoparticles are attractive materials for their applicaiton in drug, catalysts, sensors fields due to their excellent properties. Especially, the functional groups on the graphene oxide surfaces could be employed as ideal attachment regions for the metal nanoparticles. the doping of heteroatoms (N, B, S, etc.) into graphene can not only modulate the electronic structure and properties of graphene itself , but also enhance the interactions between metal, metal oxide and doped graphene. Thus, the catalytic activities and selectivities of graphene-metal nanocomposite sensors could be increased. At present, the homogenous dopant concentration on the graphene surface was achieved by in situ doping by CVD method. The advantage of CVD technique of this study the dopant will be dispersed on the graphene surface homogenously. By using NaBH4 reduction method, the synthesis of bimetallic Pd-Au catalysts was performed. The catalytic performances of these doped graphene-metal nanocomposites in terms of activity, selectivity, lifetime, and reusability was performed. As a result, it was observed that N-doped graphene supported Pd- Au catalysts is a promising electrode for glucose electrooxidation reaction

F11 - Development of New Graphene-Based Materials Containing Poly-yne Groups, For Advanced Application

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Since graphene's first isolation in 2004, it has gained overwhelming attention within academia and industry, and various publications highlight research into the covalent functionalisation of single layer graphene.[1] Unfortunately, the degree of functionalisation is often low, due to its relatively inert, conjugated system and planar structure. Much of the commercially synthesised graphene is termed "graphene", despite the fact that it often exhibits 10+ layers in thickness, and thus displays graphitic-like properties. As a result, such commercially produced graphene is at risk of possessing even lower reactivity, and hence functionalisation becomes all the more difficult.[2] The need for a functionalisation process which is facile, cost-effective and environmentally friendly, to modify these commercially produced graphene materials, becomes increasingly desirable, for large scale production of processable graphene. Herein, we present existing and proposed work relating to the covalent functionalisation of a commercially produced graphene, with the aim of tethering long poly-yne-based carbon chains to the surface. Such a synthesis process involves the formation of a suitable pre-functionalised graphene platform, which allows convenient binding to the termini of the poly-yne chain to occur. Poly-yne chains are envisioned to improve the solubility of graphene, as well as functioning as electronically conductive linkers. Potential applications of such a composite material will be investigated in due course.[3]

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F12 - Electrical properties of onion-like carbon composites

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Polymer-based composites presenting electrical percolation have attracted much attention because of the possibility to apply them as electroactive, sensitive materials, or as electromagnetic coatings [1]. It is an important to reach as-low-as possible percolation threshold in order to maintain the mechanical properties of polymers and to save the cost of expensive fillers. Onion-like carbon (OLC) as a composite filler has many advantages such as low cost, easy preparation and strong absorbtion of electromagnetic waves which leads to a potential applications for electromagnetic shielding.

In this contribution composites containing different OLC average sizes 40 nm, 100 nm and 250 nm were investigated. The electrical measurements were performed in broad frequency (20 Hz – 3 THz) range. In a frequency range 20 Hz – 1 MHz complex dielectric permittivity was measured at temperatures from 30 K to 500 K.

It was observed that the percolation threshold in composites strictly depends on OLC aggregate size. The electrical conductivity in the composites is mainly due to electron tunnelling between OLC clusters and quasi-one-dimensional hopping inside the clusters. In this presentation the impact of OLC aggregate size on broadband electromagnetic properties and the percolation threshold will be disscused.

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F13 - Nanoplatelets Enhancement of Water Barrier Properties in Polymer Nanocomposties

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Polymers with high barrier to water vapor and oxygen are a key component to various industrial applications, such as food packaging or electronic coating. Unfortunately, some polymers tend to have high permeability and therefore require loading of impermeable nanometric fillers (NF) to reduce permeability. NFs of high aspect ratio increase the diffusion path of the penetrating molecules and reduce their ability to penetrate through the material. A common barrier material for gas molecules is clay however, it swells upon the introduction of water vapor. Consequently, the permeability of the composite rises, and a degradation of other properties such as the mechanical strength occurs. In this study we investigate different approaches to the preparation of the composite: bulk and thin film, where the key filler is graphene nanoplatelets (GNP). Graphene is an allotrope of carbon possessing high electrical, thermal and mechanical properties. In addition, graphene's high aspect ratio combined with being impenetrable to most kind of gases and liquids makes it a perfect candidate for the preparation of the composite. We explore the permeability of the composite film prepared by the methods and the effect of the GNP concentration on the barrier properties. Moreover, we have investigated the effect of the NF on the mechanical properties and the thermal conductivity of the composite. The bulk preparation method resulted in a ~ 45% reduction in water vapor permeability and ~80% enhancement in fracture toughness [1], while in the thin film method provided ~80% reduction in water vapor permeability and 700% increase in the thermal conductivity. These results demonstrate the capability of GNP to enhance the barrier against WV while improving additional relevant properties for various industrial applications.

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F14 - How a nano-onion can become a sniper

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Carbon nano-onions (CNOs) are multi-shell fullerenes, structured by concentric shells of sp^2 carbon atoms.[1] These materials can be easily produced in high quantities by thermal annealing of detonation nano-diamonds. CNOs represent an interesting platform for imaging and diagnostic applications due to their spherical shape, small size, and low toxicity both *in vitro* and *in vivo.*[2]
In this work we developed a nano-carrier based on 5nm CNOs functionalized with folic acid for targeted delivery. We decorated the folic acid functionalized CNOs with a chemotherapeutic agent, doxorubicin, using a non-covalent functionalisation strategy and evaluated their specificity and cytotoxicity towards the cancer cell line HeLa CCL2. Robust characterization techniques, such as infrared and absorbance spectroscopy, thermogravimetric analysis (TGA), and X-ray photoelectron spectroscopy (XPS), confirmed the successful functionalization of the nano-carriers with the drug.
Proof of concept experiments on HeLa cells, overexpressing FR alpha (FRα), confirmed the importance of the presence of FA in the nano-carrier to selectively drive the drug inside the cells, and ultimately inducing their death. Our system, selective for and rapidly up-taken by cancer cells, can open new opportunities for the development of low-cost and biocompatible platforms capable of inducing *in vivo* selective tumor biodistribution of a drug.[3]

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F15 - Hybrid solid-state supercapacitors based on AC/MnO$_2$ cotton fabric electrodes

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One of the current trends in research in the field of supercapacitors is focused on the utilization of more flexible, low-cost and environmentally friendly materials and methods of production. Accordingly, it exists a strong interest in the integration of textiles as support of flexible, low-cost and green electrodes for wearable supercapacitors [1]. On the other hand, high surface area activated carbon (AC) based electrodes together with neutral aqueous electrolytes have been extensively studied in supercapacitors to increase their energy density and maximum operating voltage, and their capacitive limits seem that have been widely reached [2]. It is for this reason that some metal oxides with improved properties thanks to their fast reversible surface processes of faradaic type have been identified [3] and asymmetric supercapacitors made of electrodes based on AC and metal oxides have shown higher performance than the classic type of AC/AC symmetric supercapacitors. It is in this context that this work introduces some results (i. e. cyclic voltammetry, galvanostatic charge-discharge, electrochemical impendance spectroscopy, etc.) of an hybrid and asymmetric supercapacitor consisting of MnO$_2$ and AC electrodes produced with cotton fabric as starting substrate and a polymer electrolyte membrane.

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F16 - From raw to added value materials: production of carbon-based materials for gas adsorption applications as possible route for biomass valorization

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The development of technologies devoted to re-cycle and/or re-use of lignocellulosic-based wastes generated from the industrial processing of agricultural raw materials is a hot research topic [1]. Agroindustry annually generates enormous amounts of residues and their transformation from raw to added value materials as alternative to their disposal is welcome both to mitigate environmental pollution and to boost energy savings and overall cost reductions.

In a view of exploiting the advantages and shortcomings of using the materials deriving from biomass thermochemical processing as gas sorbents, in this work the gas adsorption performances of carbonaceous biomass-derived materials were tested by using various gas probes (N_2, CO_2, CH_4) exploring various temperatures (from cryogenic to near ambient conditions) and pressures (from vacuum up to ambient pressures (760 mmHg)), under equilibrium conditions. The adsorption data were analyzed and modeled in order to have a complete characterization of the textural properties of all the materials [2]. The isotherm data were also used to predict the binary mixture adsorption from the experimental pure-gas isotherms of various gas mixtures of strategic impact (ca. CO_2/CH_4, and CO_2/N_2) by applying the Ideal Adsorbed Solution Theory (IAST) [3]. The goal of the gas adsorption tests was the identification of the optimal shape, size, geometry and chemistry of the carbonaceous porous structures generated from raw biomasses as ought to be for a specific application like CO_2 capture or gas upgrading (selective absorption or ultrapure gas stream).

Three biomasses (Populus nigra wood, rice husk, cellulose fibers) and two thermochemical conversion processes (pyrolysis and carbonization) were used for the preparation of a set of samples covering a large range of chemical and textural features. Populus nigra wood and cellulose fibers were pyrolyzed under slow pyrolysis condition (5 °C/min) in presence of steam up to temperature between 480 and 700 °C, while rice husk was carbonized at 800 °C under an inert atmosphere for 3 hours. Since rice husk contains up to 20 wt.% of mineral components mostly composed of silica (87-97 wt.% of total ashes), a post-treatment with strong alkali was performed for removing this not adsorbing matter.

The analyzed biomass-derived materials exhibited a narrow microporosity with average pore sizes ranging between 0.5 and 0.6 nm allowing CO_2 and CH_4 uptakes at room temperature between 1.5-2.5 mmol/g and 0.1-0.5 mmol/g, respectively. Data showed that the samples exhibited good selectivities for CO_2 over both N_2 and CH_4.

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F17 - Novel nanocarbon design from first principles modelling and organic synthesis

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Just as it is possible to fill carbon nanotubes with fullerene molecules (so called ‘peapods’), by analogy 1:1 complexes of fullerenes with cycloparaphenylenes (CPPs)[1] have been reported, highlighting a high size selectivity of the [10]CPP to the specific fullerene C_{60}.[2]

The objective of the current work is two-fold, namely to explore different binding modes for CPPs owed to non-covalent aromatic interactions, and to manage charge-transfer processes within the self-assembled architecture (Figure 1). Towards these goals we expand the scope of encapsulating fullerene cages by CPPs by introducing the dumbbell-shaped bisazafullerene $(C_{59}N)_2$ species as an N-doped fullerene analogue of C_{60}, where a carbon atom is replaced by nitrogen.[3] Its extended length allows the capture of not one but two [10]CPP molecules, whose interaction are explored via a combination of DFT calculations, NMR measurements and UV-Vis spectra[4].

Successfully developing the fullerene encapsulation process to include different encapsulated species and multiple CPPs opens the way to different molecular machine architectures, and provides a potential templating route to CPP polymerisation. These ‘polytubes’ will represent a new carbon nanoform and could have significant functionality and advantages over conventional nanotubes, notably in composite design.

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F18 - Elastic flow instabilities and macroscopic textures in graphene oxide lyotropic liquid crystals

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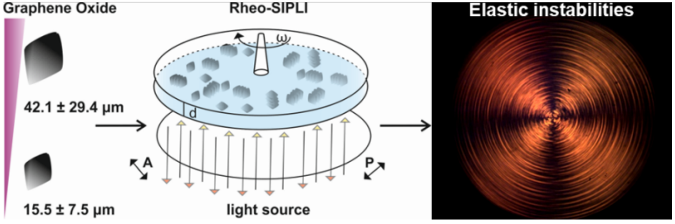
Graphene oxide (GO) is known to form a well-aligned lyotropic liquid crystal (LC) phase in aqueous dispersions at relatively low concentrations [1]. Such a system is typically charge- and sterically stabilised. It has been shown that flow and confinement conditions affect the alignment and stability of these phases [2]. A number of processes of technological relevance such as wet spinning, injection moulding or inkjet printing use GOLC inks to form graphene fibres, composites and printed conductors. We describe herein an unusual orientiation and flow patterns in GOLCs under shear-flow and confinement conditions that overlap with these processes. A helical flow arising from a combination of shear flow and Taylor-vortex type flow, resulting from elastic flow instabilities leads to a hitherto unobserved polarized light image patterns in real-time taken in situ during rheological measurements: a Maltese cross combined with shear banding (Figure 1). The unique viscoelastic properties of GOLCs of certain lateral sizes allow the elastic instabilities to occur within the theoretically predicted range of critical Deborah numbers. This may lead to advance control over desired periodic alignment of GOLCs for variety of described applications.



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F19 - Electromagnetic express non-invasive test of chloroprene rubber after long-term ultraviolet, oil immersion and thermal degradation

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The electromagnetic properties of chloroprene rubber after long-term ultraviolet ageing, oil immersion and thermal degradation were experimentally investigated in the frequency range from 1 kHz up to 1 THz. Ageing was shown in terms of mechanical degradation and the change in the complex dielectric permittivity. Within the whole investigated frequency range decrease of dielectric permittivity was observed after thermal treatment combined with oil immersion in comparison with chloroprene rubber stored under normal conditions. In contrast, thermal and ultraviolet ageing without immersion leads to increase of rubbers dielectric permittivity in all investigated frequency ranges. A non-invasive express method of degradation detection is proposed and proofed.

F20 - Synthesis of hybrid biobased conductive materials

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This paper reports the preparation of polymeric conductive materials, based on poly(lactide) (PLA)/multi-walled carbon nanotube (MWCNT) and metallic nanoparticles. For this purpose MWCNT were surface-modified by hydrochloric acid. Series of PLA/MWCNT nanocomposites, with different contents (30, 40 and 50 wt%) of functionalized MWCNT, were synthesized employing a vacuum filtration method. First, MWCNT were filtrated from water dispersion, and then PLA solution (20 wt% in dichloromethane) was poured onto MWCNT layer. After evaporation of dichloromethane elastic composite materials PLA/MWCNT were obtained. In order to increased conductivity of obtained composite, different amounts of metallic nanoparticles (zinc and aluminium oxide) 0,5; 1; and 2 wt% were added into the polymer matrix. FTIR analysis confirmed the structure of obtained samples. DSC analysis shown that a MWCNT had a significant influence on the thermal properties of obtained nanocomposites (raising the Tg and the Tm values), but addition of metallic nanofiller has no influence on the transition temperatures of obtained hybrid materials. Thermo-gravimetric analysis estimated that degradation onset temperature of composites with chemically modified MWCNT was much higher than degradation temperature of pure poly(lactide). Conductivity of obtained hybrid materials increases with increasing of metallic nanofiller contents. Highest conductivity was obtained for the hybrid materials with aluminium oxide nanoparticles.

Keywords: Hybrid material; Thermal properties; poly(lactide); MWCNT; metallic nanoparticles.

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F21 - Edge states in graphene and graphene-like materials

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According to I. Tamm and W. Shockley [1,2] electron wavefunctions can present a maximum at the surface of a material (resonance states) solely due to the fact that the structure periodicity is broken. Previous study on quasi 1D graphene-like materials such as transition metal dichalcogenide nanoribbons has shown that regardless of edge composition all structures consist of a semiconducting bulk bounded be metallic edges[3,4]. However the nature of these states is not clear yet.

In this research, we perform ab-initio calculations using Density-Functional-Theory (DFT) as implemented by the open-source package GPAW[5] and we create supercells for zig-zag graphene nanoribbons and the four representative TMD nanoribbons (MoS_2, WS_2, $MoSe_2$, WSe_2). For each structure we use a width of six unit cells at the finite y direction, and we calculate the electron probability density and the work function throughout the structures. We find that in agreement to the Shockley model, the metallic states are highly localized at the edges presenting an exponential decay outside of the nanoribbons and we are able to conclude on the width of the metallic region. Ball –and – model of the structures and the electron potential as a function of the nanoribbon width for MoS_2 and graphene nanoribbons is shown in figure 1.

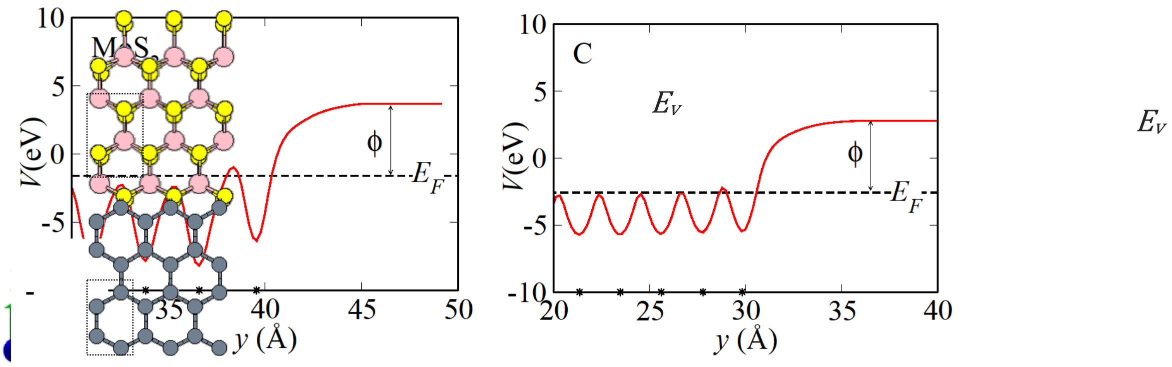

Figure 1: (left) Ball –and – stick model of graphene nanoribbons and MoS_2 nanoribbons with two chalcogen adatoms, showing two unit cells at the y direction. In TMDs pink color shows the metal atoms, while yellow presents the chalcogens. (right) Work function (ϕ) of MoS_2 and graphene nanoribbons zoomed at the upper edge. E_F is the Fermi level of the 1D structures while E_v is the electron potential in the vacuum region. The atom positions are presented with star symbols.

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F22 - Hybrid multifunctional nanostructures based on Aerographite and semiconductor materials

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Over the last years, the development of carbon based three-dimensional (3D) porous network type materials has attracted intense attention due to their high technological importance. At the same time, the fabrication of porous 3D interconnected semiconductor network structures is still limited and only few semiconductors have been synthesized as 3D networks so far.[1] This illustrates the challenges in the synthesis of 3D interconnected semiconductor networks. In our work, we use graphene aerogel and aerographite as substrates for the free growth of GaN and InP nano/micro-crystallites.[2,3] By using the hydride vapor phase epitaxy (HVPE) method, we succeeded to grow a thin layer of semiconductor nano/micro-crystallites on the Aerographite walls. GaN nano/micro-structures are very promising candidates for the next generation nanoelectronic, nanopiezotronic and photonic devices,[4] light emitting diodes and lasers, chemical and bio-sensors. The 3D porous composite material built from a network of Aerographite tubes decorated with nano/micro-crystals exhibits the fundamental features of semiconductor material as well as Aerographite. The low density, excellent electrical conductivity and mechanical flexibility of the Aerographite network along with the unique semiconductor characteristics could promote the resultant composite material, i.e., GaN-AG, as very promising candidate for various multifunctional applications, e.g., in biomedicine, 3D photonics and technologies for clean energy production. Aerographite, is a super-light weight, highly porous, graphite based 3D network material built from interconnected hollow graphite tubes having micron-scale diameters and a nanoscopic (~ 15 nm) wall thickness.[5] Note that both Aerographite and GaN are biocompatible materials,[6,7] which make them suitable for further development of smart prostheses and self-reporting artificial organs.

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F23 - Application of fractal kinetics on non-isothermal dehydration of fullerol

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Fullerols are derivatives of fullerenes with hydroxyl group on their surfaces. Due to the many of extremely important properties: radical scavengers, antioxidant, antimicrobial, anti-cancer and catalytic activity and strong electron affinity, etc. [1], fullerols found its application in a wide spectrum of scientific disciplines, of which one of the most important is in biomedical sciences [2]. Thus, understanding of interactions between fullerol molecule and water and other biofluids is of the great significance. Having this in mind, our objective is to thoroughly investigate the non-isothermal kinetics of fullerol dehydration. Non-isothermal thermogravimetric curves in temperature range from 423 K to 853 K has been recorded at different heating rates in interval from 5 K min^{-1} to 25 K min^{-1}. Thermogravimetric curves were differentiated and peak deconvolution were used in order to separate dehydration process out of other processes and reactions which occurs during thermal treatment. Complete thermogravimetric curves can be deconvoluted by three Fraser-Suzuki functions, which correspond to dehydration, dehydroxylation, and release of CO and CO2. Dehydration curves are further fitted by equation characteristic for the Brouers and Sotolongo-Costa model of fractal kinetics [4]. Dependences of rate constant on temperatures are calculated within framework of fractal kinetics model. Values of activation energy for fullerol dehydration were calculated from the dependences of rate constant on temperature using Arrhenius equation, as well as by the isoconversional method. Differences between these two approaches were discussed. Finally, activation energy distribution function were calculated. Obtained results were used to analyse changes in water structure during fullerol dehydration and can be used to define conditions under which one can obtain dehydrated fullerolls which can be further used for other aplications.

Acknowledgement
This investigation was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia trough project 172015OI

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F24 - Synthesis of doped amorphous carbon films by magnetron sputtering

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Amorphous carbon films containing oxygen and bismuth were deposited by direct current magnetron sputtering. The microstructure and optical properties of the films were measured as a function of magnetron sputtering power by atomic force microscopy, X-ray photoelectron spectroscopy, Raman spectroscopy, UV–VIS–NIR spectrophotometry, and null-ellipsometry. The oxygen concentration in the films was in the range of 19-21 at.%. It was determined that the deposition rate of amorphous carbon films increased and the surface roughness of the films changed from 1.2 nm to 1.7 nm with the increase of magnetron sputtering power. The microRaman analysis demonstrated that the D band shifted to a lower wavenumbers range and the fraction of the sp^2 carbon sites decreased as the power increased. X-ray photoelectron spectroscopy revealed that sp^3/sp^2 ratio in the films varied between 0.74 and 0.98. The optical transmission of the films in the visible region was in the range of 60-90 %. The optical band gap and the refractive index of the films depend on the dopant concentration and the sp^2 site fraction.

F25 - A photoregenerative method for low temperature NO_2 sensors

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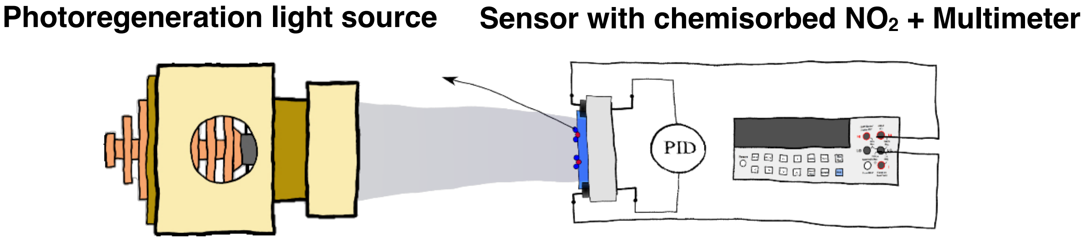
Many carbon-based materials (phthalocyanines, porphyrins, graphene, carbon nanotubes etc) are known to have high affinity to NO_2. This affinity makes them promising candidates for the fabrication of sensitive layers devoted to detect presence of this pollutant in air. However, it is also this affinity, which limits the speed of a sensor recovery process and which results in a long period of the measurement and in elevated temperatures that shorten sensor lifetimes. [1-3]
This contribution presents a robust, repeatable and low-cost method that allows to stimulate the NO_2 desorption at ambient or only mildly elevated temperatures. The method is based on short illumination of the sensitive layer by intensive UV-vis light. The method has been demonstrated on various phthalocyanines (ZnPc, CuPc and FePc) and has allowed to bring the measurement period under 2 min (from ca. 15 min, which is typical for standard operation settings). Sensor consumption has been reduced by 75%. The method requires light with a wavelength shorter than 550 nm and intensity lower than 1 mW/mm^2. Possible mechanisms of the light-stimulated desorption have been discussed. [4]
The stimulation seems to originate either in the generation of holes in the organic semiconductor that can recombine with the chemisorbed species or in the electronic transitions connected with the light absorption in chemisorbed NO_2. In any case, there have been indications that the photoregenerative method be could be transferable to other carbon-based materials.


Photoregeneration light source **Sensor with chemisorbed NO_2 + Multimeter**

Acknowledgement
This work was supported by Czech Science Foundation (GACR), Projects No. 17-13427S and No. 18-09347S and also by Ministry of Education, Youth and Sports within the projects LTC17058 and 8J18FR011 and by COST Action CA15107 MultiComp. Financial support from specific university research (MSMT No 22-SVV/2019) and PHC Barrande 2018 (40672RL) is also acknowledged.

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F26 - Comparative toxicity of carbon nanomaterials on zebrafish

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Thanks to the unique combinations of chemical and physical properties of carbon materials at the nanoscale, nowadays carbon nanomaterials (CNMs) are utilized for widespread applications in different areas as sensors, energy storage and conversion, imaging and drug delivery. All these fields and in particular the biomedical one, explicitly demand nanomaterials that are bio safe. However, data concerning the possible toxic effects of the carbon nanomaterials are still lacking. To this end, different biological models can be used to assess the CNMs nanomaterials toxicity. In this framework, zebrafish (*Danio Rerio*) represents alternative and complementary model organisms, with several peculiarities, making them established systems for toxicity screening, in comparison to other species [1]. Here, we present a detailed *in vivo* study of the bio interactions of different carbon nanomaterials, including carbon nano-onions, carbon nano-hors, nano diamonds and graphene derivatives, with zebrafish [2-3]. We assessed the CNMs toxicity at multiple levels, including mortality/survival rate as well as alterations in behavior at different stages of growth. As the use of carbon-based materials constantly increases, our results open new perspectives in the biosafety of different carbon nanomaterials.

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F27 - Films of polymer blends with tunable wettability on flat and microstructured silicon surfaces

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Carbon composites with advanced properties are very promising for novel applications and the development of smart materials. Wettability is an important property of solid surfaces governed by the chemical composition and roughness of the surface. Several applications require control of the surface wettability and especially applications of smart materials require reversible control of the wettability that can be achieved by stimuli-responsive surfaces such as polymer films. PNIPAM is a thermoresponsive polymer, which switches between hydrophilicity and hydrophobicity at 32ºC[1].

We develop thin films of blends of PNIPAM and its diblock copolymer PS-b-PNIPAM with PS (PS/PNIPAM and PS/ PS-b-PNIPAM, respectively) on flat and microstructured Si substrates and study their surface morphology and tunable wetting behavior. The morphology of the films was characterized by SEM, optical microscopy, and profilometry and their chemical homogeneity and wetting properties were characterized by Raman spectroscopy and water contact angle measurements. Films of PS/PNIPAM and PS/PS-b-PNIPAM with varying ratios and drying conditions spin casted on flat Si surfaces do not present significant changes in their contact angles below and above 32ºC. On the other hand, the effect of tunable wettability is observed for the PS/PNIPAM films, especially those with a high ratio of PNIPAM, presenting up to 25º increase of water contact angles upon heating.

The PS/PNIPAM blends, which presented thermoresponsive behavior on flat Si substrates, were tested on microstructured Si surfaces. Micro-Si surfaces were prepared by laser processing to achieve a large specific surface area with dual-scale roughness at the micro- and nanoscale. Such substrates, either with or without the native SiO_2 layer, were spin coated with PS/PNIPAM films of varying ratios. At room temperature, the micro-Si substrates provide higher water contact angles compared with the flat Si substrates. Films on micro-Si with the native SiO_2 show the highest thermoresponsivity. Films on micro-Si without SiO_2 show water contact angles up to 90º below 32ºC and up to 110º above 32ºC, becoming switchable from hydrophilic to hydrophobic upon heating. Developing micro/nanostructures with tunable wettability provides carbon composite systems suitable for several applications that require the control of wettability such as self-cleaning surfaces, industrial surface coatings, tissue engineering, cell encapsulation, sensing, and microfluidics[2].

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F28 - Synthesis and characterization of electrical conductive biocomposites from natural precursors

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Electrical conductive biocomposites are nowadays very promising as flexible electronic materials for diverse applications as biosensors or medical applications. The electrical conductivity, as well as the non-toxic nature of both matrix and filler are fundamental for these applications. The synthesis of supported graphene materials using natural precursors as sepiolite and liquid caramel by pyrolysis in the 500-800 °C temperature range has been reported [1-4]. Herein, we produced caramel-sepiolite hybrids as graphene-like precursors trying to enhance the electrical conductivity by doping with MWCNT. It is here studied the pretreatment of the caramel-sepiolite or caramel-sepiolite-MWCNT mixtures under hydrothermal conditions to promote the further carbonization of the caramel and to facilitate the next pyrolysis step necessary for the graphene-like materials generation. The structural and morphological features together the electrical properties are discussed with the aim to optimize the resulting materials which will be further incorporated into biopolymers to produce electrical conductive biocomposites.

Acknowledgement:
This work was developed within the scope of the projects: CICECO-Aveiro Institute of Materials (FCT Ref. UID /CTM /50011/2019) financed by national funds through the FCT/MEC and when appropriate co-financed by FEDER under the PT2020 Partnership Agreement. The project M-ERA-NET2/0021/2016 – BIOFOODPACK - Biocomposite Packaging for Active Preservation of Food is acknowledged for funding. CN and PF thank FCT for the grants (SFRH/BPD/100627/2014 and IF/00300/2015, respectively). This research was partially supported by COST action 15107, Grant No. 42215. We thank MINECO (Spain) support through the MAT2015-71117-R project. This work was also funded by national funds (OE), through FCT, in the scope of the framework contract foreseen in the numbers 4, 5 and 6 of the article 23, of the Decree-Law 57/2016, of August 29, changed by Law 57/2017, of July 19.

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P01 - Stronger Cement

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The growing availability of nanotubes (NT) and the increased knowledge about their loading in polymers have prompted their incorporation in cementitious matrices. The main challenge towards achieving a significant enhancement in cement properties is an effective dispersion of the agglomerated NT. In my talk I will demonstrate how efficient NT (carbon or WS_2) dispersion in cement results in substantial flexural and compressive strength enhancements at NT concentration below 0.15 wt%. The reinforcement by WS_2 NTs (see Figure 1) remains significant after a variety of curing processes, suggesting a genuine nanoscale reinforcing effect. By employing a comprehensive fractography we show that the WS_2 NTs inhibit crack propagation by bridging with a pullout failure mechanism.

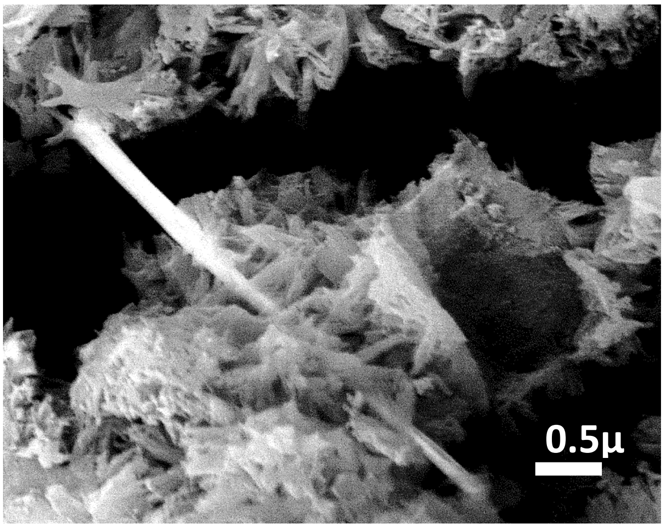

Figure 1: Scanning electron microscopy image of WS_2 NT-based cement composite showing a WS_2 NT covered by a layer of Calcium-Silicate-Hydrate (C-S-H) phase.

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P02 - Synergy effects in ferroelectric polymeric composites

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Ferroelectric polymeric materials are very attractive in various applications due to the possibility make large area, flexible and cheap devices. Ferroelectric polymeric materials can be obtained by two different ways: by producing a ferroelectric polymer or by introducing ferroelectric particles into non ferroelectric polymer matrix. The amount of wel known ferroelectric polymers is very restricted (mostly is known Polyvinylidene Fluoride (PVDF). Therefore, the second way seems to be more attractive. In this presentation the sinergy effects were investigated in both systems. First, of all epoxy resin composites with 30 wt. % of triglycine sulfate (TGS) and up to 1 wt. % of graphite nanoplatelets (GNP) were fabricated and studied by means of broadband dielectric spectroscopy (20 Hz – 3 GHz). It was demonstrated that the dielectric properties are mainly governed by the Maxwell-Wagner relaxation at lower frequencies (below 1 MHz) and by diffuse ferroelectric soft mode at higher frequencies (above 1 MHz). The ferroelectric origin of the phase transitions was also confirmed by piezoelectric investigations. Although the phase transition temperature is independent of GNP concentration, the piezoelectric and dielectric (above 1 MHz) properties of composites are strongly improved by GNP in a broad temperature range. This gives evidence for the strong synergy between GNP and ferroelectric particles. The synergy effect appears due to the better distribution of TGS particles in ternary composites and the creation of electric fields by GNP inside the composite.

P03 - Synthesis, morphology and electrochemical properties of polypyrrole nanoparticles doped with fullerene C_{60}

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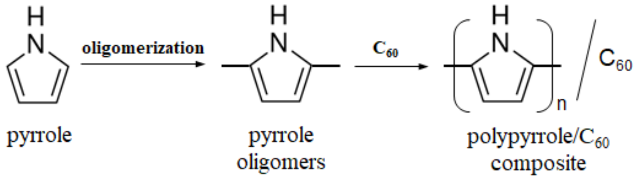
Composites of polypyrrole and fullerene C_{60} were prepared by the introduction of fullerene during polymerization of pyrrole initiated by the oxidation of pyrrole oligomers with C_{60} (Scheme 1). The rate of composite formation and its composition depend on both the component concentration in the solution used and the polarity of the solvent. Composites were precipitated in form of spherical particles and their sizes ranged from 20 to 400 nm depending on the time of polymerization. Fullerene C_{60} nanocrystals with approximate size of 1 nm were uniformly distributed within the polymeric material (Fig.1) [1].



Scheme 1. Polymerization process of pyrrole with C_{60} [1].

The amount of fullerene incorporated into polypyrrole depended on the C_{60} concentration in the solution used for the composite formation. An investigation of the composite using infrared spectroscopy indicated partial charge transfer between polypyrrole chains and fullerene nanocrystals.

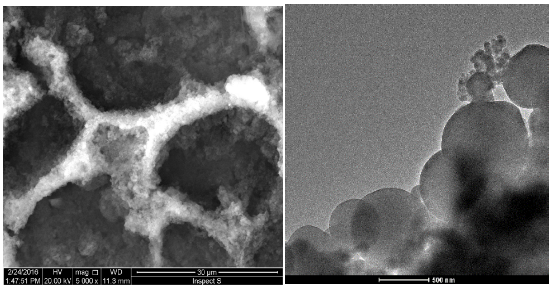


Fig. 1. SEM and TEM images of the polypyrrole/C_{60} composite from the 1,2-dichlorobenzene containing 0.1 mol·dm^{-3} pyrrole and 1.4×10^{-3} mol·dm^{-3} C_{60} [1].

The polypyrrole/C_{60} composite exhibits electrochemical activity in both the positive and negative potential ranges. At negative potentials, the fullerene nanocrystals are reduced. This process is accompanied by the incorporation of supporting electrolyte cations into the composite structure. In the positive potential range, redox processes involving polypyrrole occur. During electrooxidation of the polymeric chains, cations are removed from the composite film to maintain film neutrality.

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P04 - The benefit of carbon nanostructures addition to titanium oxide for benzene photocatalytic degradation in air

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Air pollution, in particular the emission of volatile organic compounds (VOCs), from anthropogenic sources, has significant local and global negative impacts in human [1] and environmental health [2]. Consequently, significant efforts have been made in their removal. However, VOCs when in low concentrations, are hardly degraded by a single method, due to their limited interaction with active species [3]. Thus, it is extremely desirable to develop efficient processes towards complete oxidation of low-concentrated VOCs that work in mild conditions and are energy-saving and safe [3]. Photocatalysis is a feasible methodology, as it can degrade VOCs in low concentrations [4]. Here, it is described the preparation of titanium oxide-based materials to degrade benzene as model VOC molecule. Titanium oxide (TiO_2) porous materials were prepared using an easy and environmentally friendly method followed by thermal treatments at 300 °C. Graphene oxide (GO) or carbon nanotubes (CNT) were added to TiO_2 to enhance its photocatalytic ability. The addition of carbon-based materials proved itself to be advantageous in the abatement of benzene. Additionally, samples with CNT and GO obtained better results in degrading benzene than the commercial Degussa P25.

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P05 - Hard carbon materials and their application as an anode in sodium-ion batteries

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The carbonization of rice husk results in carbonaceous materials, which are capable of Na-ions reversible storage during operation as an anode in sodium-ion batteries. The storage capacity is limited by three factors: the graphitization degree, the chemical affinity of the structure irregularities, like defects, to Na-ions, and the presence of the nanovoids, which could be filled up by Na ions. We have found that all these factors are affected by the carbonization temperature, but its extent of influence varies widely. On increasing the temperature from 900 to 1600 °C, the graphitization degree of the samples increases in terms of lateral dimension of graphene domains from 5.12 nm to 7.14 nm. The interlayer distance and the number of stacked graphene layers change only slightly. All synthesized samples are probably capable of Na ions intercalation, since graphene sheets in their regular domains are separated by a distance larger than 0.37 nm, which was reported of being necessary for Na-ions intercalation

The materials obtained at 900 °C are dense and no Na-ions diffusion was observed. For these samples the electrochemical characteristics exhibits a “supercapacitorlike” slope potential profile. The samples obtained at 1600 °C are much less compact, since they possess a lot of interconnected voids. These voids are large enough to host Na-ions and contribute significantly to the charge storage capacity. Therefore, the sample obtained at 1600 °C delivered the highest reversible capacity of 276 mAh g^{-1}. It happens mainly due to insertion of sodium ions into the nanovoids.

Acknowledgement:
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P06 - The influence of weight fraction of reduced graphene oxide on thermo-physical properties of poly(MMA/BA/HEMA) latex composites

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Due to its unique 2D structure as well as the specific properties of electrical and thermal conductivity graphene is material that has been causing the great attention of scientists in recent years. Thermal conductivity of suspended single layer graphene (around 5000 W/m K) is one of the highest thermal conductivities of currently known materials [1]. The aim of this study was to investigate the effect of weight fraction of reduced graphene oxide (rGO) (from 0.5% wt to 3 wt%) on morphological and thermos-physical properties of poly(MMA/BA/HEMA)/rGO composites. Poly(MMA/BA/HEMA) latex was synthetized by semi-continuous seeded emulsion polymerization. Reduction of graphene oxide (GO) was carried out using hydrazine. To prepare the composites by emulsion mixing technique, the aqueous dispersion of rGO and polymer latexes were mixed in different ratios to achieve final content of rGO material of 0.5, 1 and 3wt% rGO in relation to polymer. In order to determine the effect of rGO on morphological properties of composites SEM micrographs were recorded. Based on SEM micrographs, a fully organized structure was found inside the composite in which the platelets were oriented perpendicularly to the film cross-section area. The platelets are distributed between the polymer particles that hand actuated as templates around which the platelets were organizing. Thermal diffusivity of composites samples were measured using laser flash technique. The following equation $K=\alpha\rho C_p$ was used to calculate thermal conductivities of samples, where K is thermal conductivity, α is thermal diffusivity, ρ is density and C_p is specific heat capacity. Based on results linearly increasing of the values of thermal diffusivity and thermal conductivity with increase of rGO content in composites was found. The values of thermal conductivity are increased for 40% compared to net polymer, which is somewhat lower than expected, which can be explained by the uniform distribution and non-specific orientation of rGO in polymer matrices [2].

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P07 - The effects of reaction conditions on the physico-chemical and morphological properties of reduced graphen-oxide – gelatin nanocomposite hydrogels

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Hydrogels are three-dimensional networks of cross-linked hydrophilic polymers that contain a high amount of water without dissolving and have various applications However, some drawbacks, such as poor mechanical properties and toxicity restrict their applications. Polymer nano-composite hydrogels have recently attracted significant attention to overcome that. There are findings indicating the possibility of creating strong reduced graphen oxide (rGO)–gelatin nanocomposite hydrogels based on graphen oxide (GO) and gelatin, where GO acted as a reducing agent to reduce GO to rGO forming covalent bonding with rGO through its amino groups [1]. In regard to this, novel rGO–gelatin hydrogels were synthesized. In this study, a series of rGO–gelatin hydrogels at different gelatin-rGO ratios were synthesized. The effect of concentrations of gelatin solution as well as GO solution, reaction temperature and the duration of reaction on the rate of formation of composite gels, their kinetics and morphological and physico-chemical properties of the obtained composite material were investigated. The precursor of the GO – gelatin hydrogels was prepared by mixing the gelatin solution (2.4-10 % wt) and GO solution (comprising of 2-10 mg mL/L). The mixture was transferred in the glass vial and sealed, and placed in thermostat oven at different temperatures ranging from 45-95^{o}C, in time intervals from 1-24 hours. The obtained reaction products were lyophilised. The gelling time was determined by visually method. The Fourier transform infrared spectroscopy (FT-IR) was carried out on a Perkin Elmer Spectrum 100 Spectrometer. The analysis of samples surface was performed by using scanning electron microscopy (JEOL JSM-840A). All samples were gold sputtered in a JFC 110 ion stutterer. The hermogravimetric (TG) curves of non-isothermal degradation under nitrogen atmosphere have been recorded using a TG Analyser, TA Instruments . Based on the obtained results the following was concluded. The gelatin-rGO nanocomposites were formed within temperature range 65^{o}C - 95^{o}C and time interval 4h - 8h. The gelation reduced GO entirely into rGO. The rGO in the forms of nano-sheets is uniformly dispersed in the formed composite. The swelling degree of the synthesised composites varies from 1-70 g/g, depending on the reaction conditions. The thermal stability of gelatin-rGO nanocomposites is significantly improved in comparison to pure gelatin based hydrogels.

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P08 - Formation of amorphous carbon films using Ar-C_2H_2 and Ar-C_2H_2-H_2 plasma

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Amorphous carbon films have attracted considerable interest due to their wide range of excellent properties. Those properties make amorphous carbon films suitable for a large variety of application fields such as: tribology, microelectronics, biomedicine, energy, optics, and etc. Nowadays a considerable attention is given to the formation of amorphous carbon films at atmospheric pressure. The main advantage of such process is the possibility to replace a high cost vacuum system by plasma equipment which can be operated simply at air conditions.

Amorphous carbon films were formed on the silicon-metal substrates at atmospheric pressure using a linear direct current plasma torch. A thin metal layers were deposited on Si substrate by magnetron sputtering technique. Argon or argon-hydrogen mixture was the plasma forming gases. Acetylene (C_2H_2) gas was used as carbon source. Argon-acetylene and argon-hydrogen–acetylene plasma were studied in the range of 250–800 nm wavelength using an acousto-optic emission spectrometer (OES) IFU AOS4. The surface morphology, elemental composition and bonding structure of the amorphous carbon films was investigated by scanning electron microscopy (SEM), energy dispersive X-ray (EDX), Raman scattering spectroscopy (RS) and Fourier transform infrared (FTIR) spectrometer. Nanoindentation tests were performed by MTS-Agilent G200 nanoindenter. OES measurements indicated that the C_2 and CH species are dominated in the argon-hydrogen-acetylene and argon-acetylene plasmas. The introduction of the hydrogen into the plasma reduces the fraction of C_2 species in the plasma. The bonding structure and oxygen content in the films strongly depend on the hydrogen content and deposition temperature. The Raman measurements indicated that films deposited using argon-acetylene plasma were amorphous carbon with nanocrystalline/glassy carbon phase. Microhardness and Young's modulus values significantly depended on the plasma composition and formation distance.

P09 - Deep eutectic solvent/carbon materials interfacial studies for potential energy storage applications – Effect of carbon modification

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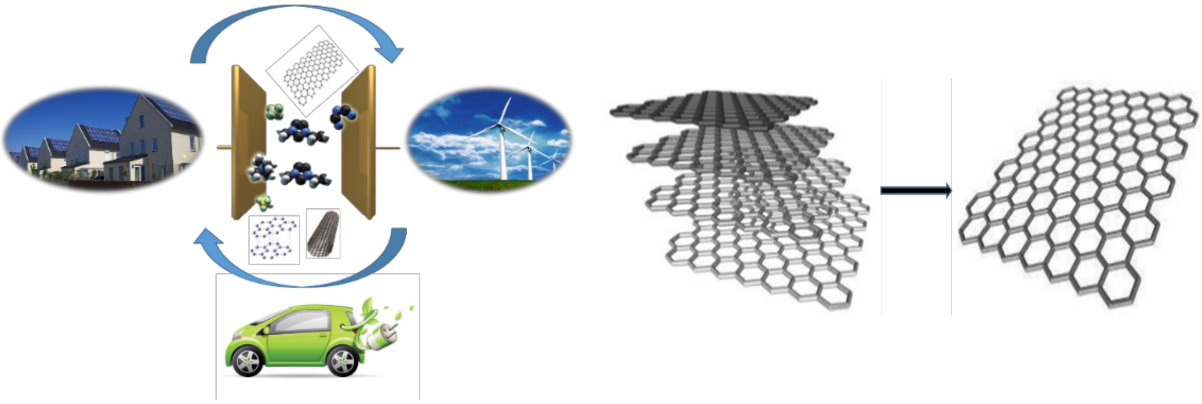
Renewable Energy, coupled with energy efficiency improvements are key elements for the Global Energy Transition Roadmap in bringing a sustainable, safe and smart energy future [1]. Accordingly, supercapacitors are drawing deep attention as high-performance energy storage devices for high energy demand applications. Energy storage is a very challenging topic that may enclose complex mechanisms occurring during the energy harvesting, conversion and storage steps.

In this work, we present recent results that may contribute to a new generation of electrodes based on carbon materials with the potential application on supercapacitors. Specific capacitance was measured for graphene, graphite and structurally changed graphite/glassy carbon composite electrodes in contact with choline chloride: ethylene glycol (1:2) deep eutectic solvent. Stability was followed by measuring charge/discharge curves at different current densities. CV analysis was also performed.



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P10 - Controlling Microstructure in Nanocomposites using Magnetic Fields

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The microstructure of nanocomposites is fundamental to their bulk properties. For mechanical reinforcement lower volume fractions with high levels of dispersion are desirable. Whereas for thermal or electrical conductivity percolated networks, with higher filler loadings are required and some agglomeration can be beneficial. This makes the achievement of nanocomposites with enhanced mechanical and functional properties challenging. In pursuit of a better balance of properties researchers have adopted a range of approaches to controlling the microstructure of nanocomposites. Such as freeze casting, emulsion casting, templating and self-assembly [1-4]. Whilst improvements in properties such as conductivity at low volume fractions have been demonstrated, these approaches are not readily scalable and lack control or the ability to select and achieve a desired structure. The use of externally applied fields is an alternative approach where predominantly electrical and magnetic fields are utilized to align and structure nanomaterials. The scalability of these approaches can also be limited, particularly as the low magnetic susceptibility of nanocarbons means that very high magnetic fields have been required (15-25T [5]).

In this work we adopt a co-precipitation approach to decorate graphene flakes with magnetite (Fe_3O_4) nanoparticles (<40nm diameter). Extensive chemical characterization using XPS, Raman, SEM, TEM and diffraction has been undertaken to confirm the morphology and allotropic form of these particle. We have increased the magnetic susceptibility of graphene from 0.035 for 29.58 emu/g (measured using VSM). We have shown that these materials can be manipulated within an epoxy resin at very low magnetic field strengths (<100mT). The alignment of graphene flakes is demonstrated through optical microscopy, SEM and Small Angle X-ray Scattering (SAXS). We study the limit of magnetic actuation and the variation in achievable microstructures and correlate this to final composite properties (thermal and mechanical).

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P11 - Graphene flakes dispersed in polycarbonate: thin films composites and optical properties

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Single layer graphene, with carbon atoms arranged in a hexagonal lattice, is a 2D material with sp^2 electronic structure exhibiting, among the others, peculiar optical[1] and electrical properties[2]. The strong interest in the physical properties of this material and of similar ones, such as few layer graphene obtained by exfoliation or single layers of 2D transition methal dichalcogenides, has triggered widespread use in a variety of fields. Among the potential applications, graphene flakes can be used as the fillers in polymers to form new composites. We focused on composites with polycarbonate matrix. Graphene flakes dispersed in a proper solvent were mixed with a polycarbonate solution to achieve an intimate contact between fillers and matrix polymer chains. We used the casting technique from solutions made using a chlorinated solvent. Composite films were made using three different loadings in the range of 0.5-2wt%, and it was observed that there was no loss of transparency up to 3 wt% loading. Furthermore, the concentration of polycarbonate was changed, to obtain different film thicknesses. Additionally, the conductive graphene flakes can also result in electrical discharging of the polycarbonate surface. This could solve some common problems of lightning strike dissipation in aircrafts, which can cause serious effects such as the damage of electric circuits. The composite films were prepared and characterized by Raman and IR spectroscopy, X-ray diffraction, and SEM imaging. The graphene flakes showed inert chemically structure with low impact on the polycarbonate chains, without inducing a significant change on the amorphous or crystalline state. Thus, graphene strengthens the polymer without inducing the growth of crystals phase, different from e.g. gold nanoparticles. SEM showed that the films made had good homogeneity, without loss transparency, translucent effects or lumps as electron dense zone. Thanks to the different composite film thicknesses, different film absorption and thus optical response was obtained. No aggregation was observed and the optical quality of thin films was good up to 87% in transparency.

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P12 - Surface effects of sintered steel processed by material extrusion

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Additive manufacturing became a manufacturing tool covering vast industrial branches. It's reach is only limited by the materials which can be used by each manufacturing method. One of the most accesible manufacturing methods is material extrusion by using filaments as a feedstock material. The variety of materials, that can be used to produce components, results in a wide variety of application potentials. A new branch in the usage of materials is taken from metallic injection moulding, where polymer feedstock is filled with steel particels. The mixture can take up to 80 weight per cent, resulting in a high filled green body. By varying the the mixture from injection moulding applications to material extrusion, completely new geometries can be realized. Since material extrusion is not a technology to produce high part quantities, the following steps in part creation, the debinding and sintering process, are normally quite costly. Most of these costs come from sintering the steel particles in a hydrogen atmosphere. To avoid chemical reactions with oxygen, a number of security steps need to be taken, resulting in costly sensor and prohibition equipment. By using a process gas, these costs can be reduced to a minimum. Still the atmosphere has an influence on the resulting surface properties, which will be presented.

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P13 - Spectroscopic study on Eumelanin / Graphene-like hybrids by nuclear magnetic resonance and photoemission spectroscopy

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Eumelanin-based blends obtained integrating such pigment with organic conducting materials are opening new perspectives in the field of bioelectronics. Among these, our recent works on hybrid materials obtained from eumelanin and graphene-like (GL) layers revealed how they are promising as concerns biocompatibility and transport properties [1-2]. However, a limiting factor for the implementation of eumelanin-based electronic devices comes from the low absolute value of conductivity of the pigment, and from the fact that the conduction mechanisms are still matter of debate. A major goal lays therefore in the knowledge and feasible control of structure/properties relationship, in order to reproducibly achieve the desired electrical and structural properties. In this respect, advanced spectroscopic techniques such as nuclear magnetic resonance (NMR) and synchrotron-based techniques, offer a unique possibility to perform deep investigation on electronic and structural properties of complex hybrid compounds. We prepared different hybrid materials by in situ polymerization of the eumelanin precursor DHI in presence of various amounts of GL layers. Solid state NMR data indicated that structural and packing modification occurs in the hybrids with respect to eumelanin. Resonant photoemission spectroscopy measurements supported this observation, giving evidence of a stronger interaction, in the hybrids, of the single atom with the surrounding environment through the observation of a faster delocalization mechanism. These findings demonstrate the impact of the integration of GL on the structural organization of the pigment, even with negligible changes in terms of chemical units (as revealed by infrared and photoemission spectroscopies). By comparing the spectroscopic results with electrical measurements, it appears that a tighter packing of the constituent units could represent the key to elucidate the improved electrical conductivity of the hybrid materials, and could be exploited as a tool for electrical conductivity tuning.

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P14 - Electronic structure of Two-Dimensional Conjugated Microporous Polymers

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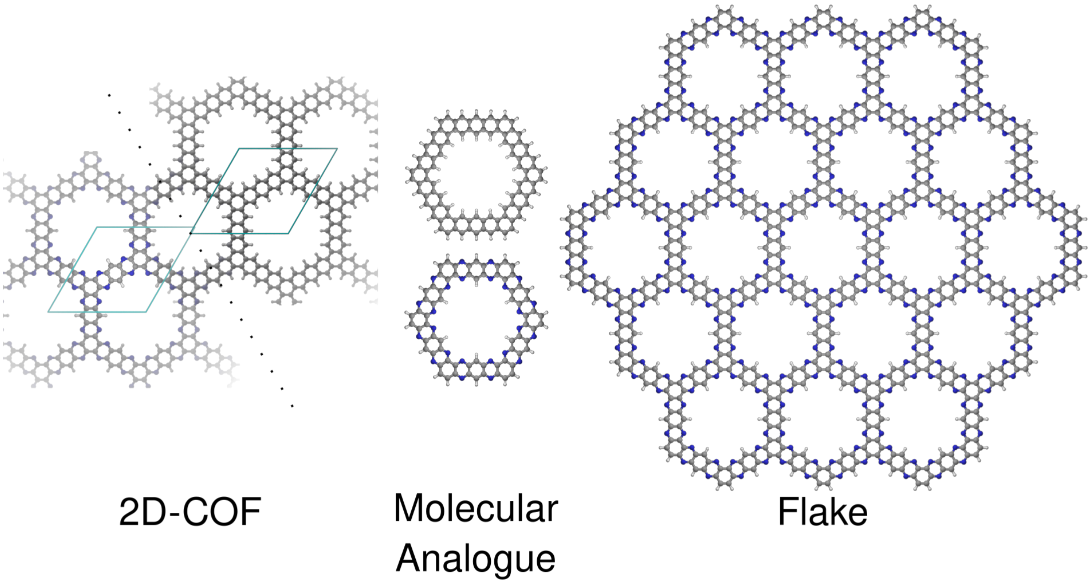
Covalent Organic Frameworks (COFs) that are readily dispersible in solvents were recently synthesized and studied[1,2]. Computational studies of the full series of crystalline of 2D Covalent Organic Frameworks based on these systems[1] together with several molecular analogues were performed. The objective was to understand how the variation of the pore size alters the electronic properties. Initial studies indicates that structures with pores > 10 nm are feasible.[3]



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P15 - Effect of Graphene Nanoplatelets in the dynamic crystallization of PEEK

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Poly ether ether ketone (PEEK) is a high performance thermoplastic polymer with relevant properties such as high thermal stability and high melting temperature. PEEK is semicrystalline polymer and its physical and mechanical properties depend on the crystalline morphology as well as the crystallinity, both highly sensitive to processing conditions and additives[1]. The crystallization of PEEK can be affected by the addition of nanofillers. Because they may influence the crystallization process such as in the nucleation as in the crystal growth. During the nucleation, nanofiller can act as nucleating agent promoting heterogeneous nucleation, increasing crystallization rate among others factors. During the growth of crystallites, nanofillers could restrict the mobility of the polymer chains, reducing the crystallization growth rate. Graphene nanoplatelets (GNP), which are formed of several layers of graphene, have attracted the attention of the scientific (academic and industrial) community, because they have a good balance between some properties of graphene and their ease and low cost production compared to pristine graphene[2]. The effect of GNP in the crystallization of PEEK is still unclear due to the few studies available in the literature and this is the main aim of this work.

The effect of the graphene nanoplateletets (GNP), at concentration of 1, 5 and 10 wt.%, in PEEK composite dynamic crystallization from melt were investigated by DSC and real time X-Ray diffraction experiments. DSC results showed a double effect of GNP: a) nucleating effect crystallization from melt started at higher temperatures and, b) longer global crystallization time due to the reduced polymer mobility. This hindered mobility were proved by rheological behavior of nanocomposites, because to the increase of complex viscosity, G', G'' with the GNP content. Finally, real time WAXS/SAXS X-Ray measurements proved that GNP has not affected the orthorhombic phase of PEEK nor the evolution of the crystal phase during the crystallization processes. However, the correlation length of the crystal obtained by WAXS and the long period (L) by SAXS varied depending on the GNP content[3].

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P16 - Effect of morphological structure on physical properties of SWCNT/PE nanocomposites

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Polymer nanocomposites with carbon nanotubes (CNT) have been a topic of extended research for about 20 years. While literature shows effects of CNT based factors (CNT type, geometry, chirality, etc.) as well as CNT-polymer based factors (functionalization, processing technique, matrix materials, etc.) on physical properties of nanocomposites, our goal was to evaluate, how morphological structure of matrix material (linear or branched) affect the performance of nanocomposites in a view of rheological, mechanical and thermal properties.

Within the scope of our research, industrial grade single-walled carbon nanotubes (SWCNT) were mixed with low-density polyethylene matrix (LDPE-branched structure) as well as with high-density polyethylene matrix (HDPE-linear structure). SWCNT was obtained in the form of masterbatch, i.e. Tuball 801 (OCSiAl, Luxembourg) with 10 wt.% of SWCNT dispersed in polyethylene wax, while following matrix material were used, i.e. LDPE (780 E NATURAL, Dow Chemicals Company, USA) and HDPE (HDI2061 NATURAL, Braskem IDESA, Mexico). SWCNT masterbatch was mixed in high- and low-density polyethylene using Minilab micro-compounder equipped with MiniJet injection molding machine. The temperature of compounding was 220 °C, time of mixing was 10 minutes, screw speed was 200 rpm, injection molding pressure was 500 bar, mold temperature was 45°C and the SWCNT concentration was spanned from 0 to 1 wt.%.

Rheological characterization, i.e. flow tests, were performed by a rotational rheometer (Anton Paar, MCR 320, Austria) at constant temperature 150°C in shear stress range from 0 Pa to 10^4 Pa. Results show that with the addition of 1wt. % of SWCNT the zero-shear viscosity increases for LDPE approx. 3,5 (300%) and for HDPE approx. 7 (700%) times compared to the neat matrix material, which demonstrates the formation of CNT-network with percolation threshold at approx. 0,3 wt.% of SWCNT content for both materials.

Mechanical characterization, i.e. tensile tests, were performed in universal testing machine (Shimadzu, AG-X, Japan). The influence of SWCNT on tensile modulus was higher for the LDPE than for the HDPE, where tensile modulus increases for 260% and 30% respectively with addition of 1 wt.% of SWCNT.

Thermal properties were determined by a Mettler Toledo DSC1 differential scanning calorimeter. SWCNT acted as a weak nucleating agent for crystallization of LDPE and HDPE. However, the stronger influence was observed for HDPE. For both polymers, the crystallization started at a higher temperature and the rate of crystallization was lower. Therefore, the crystallization proceeded in a broader temperature range and the enthalpy of crystallization was decreasing with increasing SWCNT concentration.

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P17 - Photodegradation of RhB by functionalized MoS2 sheets and coreshell Ag@Au nanoclusters

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Driven by global environmental degradation, renewable photocatalytic solar energy conversion schemes hold great promise as alternative technologies for the removal of contaminant molecules such as organic dyes from wastewater. In this context, the development of novel donor-acceptor ensembles is mandatory, as they can efficiently harvest solar energy, convert it into charge carriers allowing the occurrence of controlled electron transfer reactions.

Herein, we investigate the photocatalytic properties of water-soluble nanoensembles based on gold (as core) and silver (as shell) metal nanoclusters, abbreviated as Ag@AuNCs, and ammonium functionalized MoS2 sheets (abbreviated as f-MoS2). Briefly, Ag@AuNCs labeled with bovine serum albumin (BSA) bearing negative charges at alkaline media and f-MoS2 possessing positive charges attributed to the presence of ammonium units on their skeleton, were electrostatically coupled. The successful fabrication of the Ag@AuNCs/f-MoS2 hybrid was manifested with the aid of absorption and photoluminescence titration assays. Markedly, with the latter the fluorescence quenching of Ag@AuNCs upon incremental additions f-MoS2 revealed the development of electronic interactions between the two species at the excited states. Next, the photocatalytic activity of Ag@AuNCs/f-MoS2 was assessed by monitoring the degradation of Rhodamine B (RhB) through spectral changes in the absorption spectrum of the dye. The photodegradation of RhB by Ag@AuNCs/f-MoS2 followed fast kinetics as compared to that of bare Ag@AuNCs or individual AuNCs and AgNCs highlighting the important role of MoS2 as electron acceptor for the catalytic reaction. Furthermore, charge-transfer phenomena were witnessed within Ag@AuNCs/f-MoS2, with the production of highly oxidant radicals being responsible for the photocatalytic degradation of RhB, while on an additional path, photogenerated holes on Ag@AuNCs can also directly attack and degrade the dye.

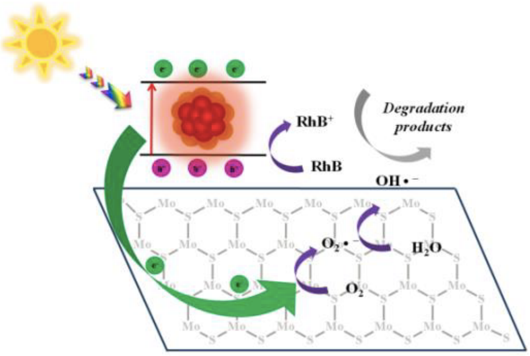

Figure 1. Illustration of the mechanism for the photodegradation of RhB by Ag@AuNCs/f-MoS2 hybrid

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P18 - Pd@M (M=Ni, Cu, Co) nanoparticles / graphene ensembles toward the oxygen electroreduction

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The world's rapidly growing demand for energy along with the depletion of fossil fuel reserves renders the exploration of new environmentally friendly energy sources an urgent issue. Fuel cells, based on potentially renewable fuels, have attracted considerable attention as the most promising power sources for portable electronic devices and transportation vehicles due to their high energy conversion efficiency. The most important cathodic reaction involved in fuel cells is the oxygen reduction reaction (ORR). However, ORR is kinetically challenging as characterized by sluggish kinetics, rendering the incorporation of catalysts in the fuel cell device to improve activity. Currently, platinum and its alloys are commonly employed to catalyze ORR. Recent efforts are focused on replacing Pt owed to its prohibitively high cost, and limited durability in the harsh reaction conditions. Thus, the reduction of total precious metal loading in an oxygen reduction cathode electrocatalyst without sacrificing performance is regarded as a core challenge for the successful commercialization of the fuel cell technology.[1-2]

In this study, Pd@M (M= Ni, Cu, Co) nanoparticles with core-shell morphology, interfaced with non-covalently modified graphene sheets were prepared via a two–step methodology and examined as novel electrocatalysts toward the ORR. High resolution and scanning transition electron microscopy, HR-TEM and STEM, respectively, while their elemental composition was probed via energy dispersive spectroscopy (EDS) and electron energy loss spectroscopy (EELS) chemical mapping to investigate the morphology of the $Pd@M_{NPs}/G$ ensembles. Complementary spectroscopic techniques, comprising Raman, UV-Vis and photoluminesce (PL) spectroscopy, were also involved for the complete their physical characterization. Detailed investigation of their electrocatalytic performance toward ORR was achieved through rotating disk electrode voltammetry, followed by the Koutecky – Levich analysis to identify the exact reaction kinetics. Finally, chronoamperometric tests were performed to assess their long-term stability. The results suggested that the optimum electrocatalyst was more active for the ORR in alkaline environment than the benchmark Pd/C catalyst, albeit with significantly lower precious metal loading, rendering it a viable alternative for energy conversion applications.

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P19 - Adsorption, Kinetics, and Bundle Size Distribution as Determining Factors in Surfactant-Assisted Dispersions of Carbon Nanotubes

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Dispersing single-walled carbon nanotubes (SWNTs) in water is essential for many applications. In noncovalent methods, the hydrophobic moiety of the dispersant adsorbs on the SWNTs, while the hydrophilic part interacts with the solvent, conferring colloidal stability to the SWNTs.[1] However, the whole dispersing process is not totally understood and several questions, such as the requirement of a minimum dispersant concentration to suspend sizeable amounts of SWNT, or the origin of the different SWNTs maximum dispersibility plateau obtained for different dispersants, remain open.[2,3]

To get further insight, we produced aqueous dispersions of pristine SWNTs using an amphiphilic triblock copolymer (Pluronic F127) as dispersant. Upon centrifugation, one obtains a dispersion with suspended individual tubes and thin bundles. In the final dispersion, we determined the dispersed SWNT amount, the dispersant concentration and the fraction adsorbed at the SWNT surface. Sigmoidal dispersion curves recording the concentration of dispersed SWNTs as a function of supernatant dispersant concentration were obtained at different SWNT loadings and sonication times.[3]

As SWNT bundles are debundled into smaller and smaller ones, the essential role of the dispersant is to sufficiently quickly cover the freshly exposed surfaces created by shear forces induced during sonication. Primarily kinetic reasons are behind the need for dispersant concentrations required to reach a substantial SWNT concentration. Centrifugation sets the size threshold below which SWNT particles are retained in the dispersion and consequently determines the SWNT concentration as a function of sonication time.[3]

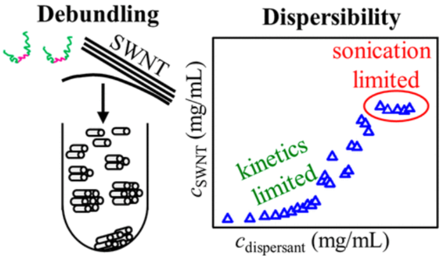

Figure 1. Schematics of the dispersing process: at low dispersant concentration the SWNT dispersed is limited by the adsorption kinetics while at the plateau is limited by the applied sonication and centrifugation parameters.

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P20 - Comparing the dispersibility of carbon nanotubes and graphene using amphiphilic molecules: similarities, differences and trends

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In recent years, carbon nanotubes (CNT) and graphene have become exciting nanomaterials for a wide range of applications.[1-2] Because of their 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. In this work, we have developed and explored a methodology to exfoliate carbon nanotube bundles and graphite in aqueous surfactant solution under well-controlled conditions. From the profile of the dispersibility curves, several quantitative parameters were extracted, which altogether permit reliable comparisons between different surfactants.[3-5] Further, the exfoliated materials were characterized by AFM and SEM, allowing the determination of the CNT individualization degree and the content of few-layer graphene in the dispersions. Additionally, graphene nanoplatelets were dispersed, allowing further insight on the surfactant role in the dispersion of these nanomaterials. This work contributes to a systematic investigation on the mechanisms of surfactant-assisted exfoliation of 1D and 2D carbon nanomaterials, 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.

Acknowledgement

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P21 - Gemini surfactants as efficient dispersants of multiwalled carbon nanotubes

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Surfactants have been widely employed to debundle, disperse and stabilize carbon nanotubes (CNTs) in aqueous solvents. Yet, a thorough understanding of the dispersing mechanisms at molecular level is still warranted [1]. Herein, we investigated the influence of the molecular structure of gemini surfactants on the dispersibility of multiwalled carbon nanotubes (MWNTs). We used dicationic *n-s-n* gemini surfactants, varying systematically *n* and *s*, the number of alkyl tail and alkyl spacer carbons, respectively; for comparisons, single-tailed surfactant homologues were also studied [2-4]. Detailed curves of dispersed CNT vs. surfactant concentration were obtained through a stringently controlled experimental procedure, allowing for molecular insight: the gemini are found to be much more efficient dispersants than their single-tailed homologues, i.e. lower surfactant concentration is needed to attain maximum dispersed CNT concentration; in general, the spacer length is comparatively more influential than the tail length in dispersing efficiency; our observations also point to an adsorption process that does not entail the formation of micelle-like aggregates on the nanotube surface but rather coverage by individual molecules. SEM imaging shows a sizeable degree of CNT debundling by the gemini surfactans in the as-obtained dispersions. These studies are of great interest for the rational choice of optimal dispersants for carbon nanomaterials and similar insoluble anisotropic materials.

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P22 - Tuning carbon nano onions for CO_2 capture

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The concentration of CO_2 in the atmosphere has been increasing during the last decades due to the human activities and it is causing global warming [1-2]. The European Union's targets for 2030 are to reduce by 40% the CO_2 emissions [1]. The capture, storage and reuse of CO_2 is one of the main strategies to reduce the CO_2 release in the atmosphere. Different technologies are proposed for the CO_2 removal, such as adsorption, absorption, membranes and cryogenic processes. The former method has some advantages when compared with other processes in terms of operation costs and adsorbent reusability [1-2]. However, this methodology still commercially unavailable due to the lack of effective adsorbents that can be used for this propose. Thus, the design of a cost-efficient and sustainable effective adsorbent for CO_2 removal needs to be explored [2]. Carbon nano-onions (CNOs) are high conductive materials that due to its moderate external surface area (200-600 $m^2 \cdot g^{-1}$), a large number of mesopores (between 2 and 50 nm) [3], easy preparation and scalability seems to be a promising solution in the CO_2 capture. Moreover, this kind of materials can be chemically functionalized in order to improve their interaction with the CO_2 molecules [4].

Here, we describe the preparation of amine-modified CNOs as feasible adsorbents for the CO_2 adsorption. The CNOs were prepared by thermal annealing of nano-diamonds at 1650 °C under an inert atmosphere [5]. After CNOs' oxidation, amino groups were introduced onto the CNOs surface via grafting of an amino-silylated precursor or via amidation reaction using a diamine precursor. The resulting amino modified CNOs adsorbents have enhanced CO_2 adsorption comparing with the pristine material.

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P23 - DFT investigations of 3D C_{60} polymers with ordered binary-alloy type structures

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Three-dimensional (3D) C_{60} polymerized structures with each molecule adopting one of the two standard orientations, have been studied via density functional theory methods (DFT). The structures investigated were constructed using, as prototypes, well-known ordered binary-alloy (AB) structures - AuCuI, Au_3Cu, CuPt, "A_2B_2" - , in which one standard orientation corresponds to atom A and the other orientation corresponds to atom B. We show that in all the studied structures 56/56 2+2 cycloaddition polymeric bonds are formed between differently oriented molecules but not between similarly oriented molecules. It, thus, corresponds to an orientational antiferromagnetic interaction and the system can be mapped onto Ising fcc antiferromagnet [1]. The bonding type, 56/56 2+2 cycloaddition, is different from the 66/66 2+2 cycloaddition characteristic of the low-dimensional, 1D and 2D, C_{60} polymers, as it is formed between intramolecular single bonds of neighboring molecules and not between intramolecular double bonds.
The electronic and elastic properties of such polymeric structures were also calculated, at room pressure and at 9.5 GPa. All these structures show metallic behavior [2].

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P24 - Roots towards innovation in sustainable poly(2,5-furandicarboxylate)s polymeric materials

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The issue of plastics is raising serious concern among scientists and the society at large. In fact, it is calculated that since the late 1950s' the total volume of polymers ever produced is 8.3 billion metric tons.[1] A realistic scenario points out that 5 billion metric tons are now accumulated in the landfills or the natural environment because they were prepared under the paradigm of stability, and not to be biodegrade. Additionally, they were/are based on fossil resources. In this context, this study tackles the demand for (bio-)degradable polymers derived from renewable-resources, but still having high-performance thermal and mechanical properties. In this study, 2,5-furandicarboxylic acid (FDCA) (or its di-methyl derivative) and different comonomers (*e.g.* poly(ethylene glycol) (PEG), poly(lactic acid) (PLA), 1,20-eicosanediol (M20), diglycolic acid), were used to prepare fully renewable polymers, namely the poly(1,4-butylene 2,5-furandicarboxylate)-co-poly((poly(ethylene glycol)) 2,5-furandicarboxylate) (PBF-co-PEGF),[2] poly(butylene 2,5-furandicarboxylate)-co-(butylene diglycolate)[3] copoly(ester(ether))s; poly(ethylene 2,5-furandicarboxylate)-co-poly(lactic acid) (PEF-co-PLAs)[4] copolyesters; poly(1,20-eicosanediyl 2,5-furandicarboxylate) (PM20F) homopolyester,[5] among others. These polymers have both stiff aromatic-like units introduced by FDCA and soft aliphatic moieties due to the aliphatic comonomers used, thus modulating, the glass transition and melting temperatures, along with (bio-)degradation and hydrophobicity behaviour of the new materials.

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P25 - The Nano-patterning of Two-dimensional Atomic Structures by Focused Ion Beam Treatment

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The nano-patterning of nanostructures for two-dimensional device application is actual. The focused ion beam (FIB) is a powerful technique for modification of nanostructures (from a few to many layers) for nanodevice application. The aim of this work is to modify the bulk nanostructures (nanowires), nano-pattern two-dimensional materials (graphene, hexagonal boron nitride and their hybrid stacks [1]) and fabricate scanning tunnelling microscope (STM) tips using a Ga^+ FIB. For that reason the FIB source together with a scanning electron microscope (SEM) gun was used. The ion bombardments were performed using a Ga^+ ion source working at 30 keV accelerating energy, with an ion current of a few picoamps (for two-dimensional materials) and a few nanoamps (both for nanowires and STM tips) at different bombardments times (few to hundred nanoseconds). SEM and STM were used to register the changes caused by nano-patterning processes after FIB treatment. The surface patterning on graphene and other two-dimensional material sheets and their hybrid stacks were performed [1, 2] using a focused gallium ion beam. The nano-patterning of a few layer graphene were performed without mask or resist. The optimum conditions for irradiation were revealed, which allowed performing ion bombardments with low damage. The FIB polishing allows clarifying how homogeneous the bulk nanostructures (nanowires) are. After epitaxial growth dark spots and surface features of the nanowires arise. The FIB polishing allows clarifying if they are really just surface features. The FIB milling gives information on the deeper interior of the nanowires, i.e. buried structures within the nanowires and whether those structures propagate within the nanowires. The FIB treatment of two-dimensional atomic materials opens promising perspectives for modifications of the nanostructures for nanodevice application.

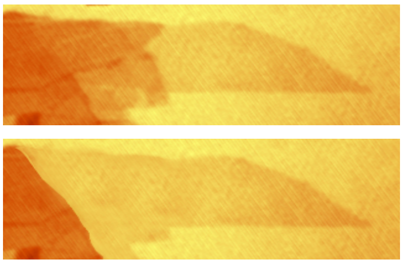

Fig. 1. Optical images (100x magnification) of graphene samples:
a) as-prepared few and multiple layer graphene sample made by Scotch tape method before FIB treatment (upper image),
b) monolayer graphene sample after FIB treatment (lower image).

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P26 - Pulmonary toxicity of inhaled graphene-based nanoplatelets

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Graphene-family nanomaterials (GFNs) have unique physicochemical properties such as great electrical and thermal conductivity or strong mechanical strength, thus having enormous potential for a wide set of applications in several fields. However, the widespread use of GFNs is raising great concern regarding their potential impact on human health. This is particular relevant in a scenario of occupational and environmental exposures where pulmonary toxicity may occur. Herein, we performed an *in vivo* based study, in which we investigated the pulmonary toxicity of single layered graphene (SLG), graphene nanoplatelets (GNPs) and carbon black (CB). Wistar rats were exposed by inhalation for 4 weeks to different concentrations of GFNs and sacrificed after 3 and 28 days of recovery. Bronchoalveolar lavage fluid (BALF) cells were collected and cell cycle dynamics profile was analysed. Furthermore, Nuclear Magnetic Resonance (NMR) metabolomics was applied to unveil pulmonary metabolic variations. The results showed that all materials induced alterations in the cell cycle of BALF cells. SLG and CB induced an increase in the sub G0/G1 subpopulation, which may indicate DNA damage. Furthermore, SLG induced a dose dependent decrease in the percentage of cells at G0/G1 and an increase in the percentage of cells in S-phase, which was mostly maintained after the 28-days recovery period. On the other hand, GNP exposure did not induced changes in the cell cycle dynamics of BAL cells. NMR metabolomics of intact lung tissues revealed that both SLG, GNP and CB exposures induced alterations to the normal metabolic profile of the rat lungs, mostly related to antioxidant pathways.

P27 - Regioselective Synthesis of an *Equatorial*$_{face}$ Bisadduct of Azafullerene. Molecular manipulation towards efficient fullerene-based electron acceptors.

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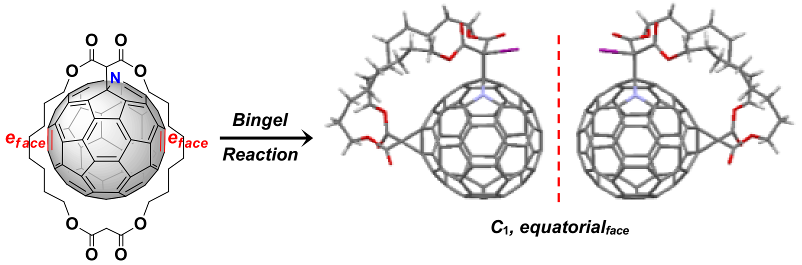
Nowadays the chemistry and applications of bisazafullerene $(C_{59}N)_2$ receives increasing attention.[1] Starting from commercially available C_{60}, $(C_{59}N)_2$ can be obtained in a three-step reaction sequence with an overall yield exceeding 10%.[2] This allows the acquisition of sub-gram quantities in short time scale, allowing to perform extensive studies with $(C_{59}N)_2$.

We have synthesized and fully characterized the first bisadduct of heterofullerene $C_{59}N$, exploiting a tether-directed remote functionalization strategy.[3] *Cyclo*-[2]-octylmalonate tether was added on the $C_{59}N$ cage via a Mannich-type reaction,[4] followed by an intramolecular iodine-catalyzed Bingel cyclopropanation reaction, which afforded a single bisadduct. ^{13}C NMR spectroscopy unveiled the C_1 symmetry of the formed bisadduct, while X-ray single crystal analysis revealed an *equatorial*$_{face}$ addition pattern. Bisadduct **(±)-3** has distinct absorption features, which constitute signatures for the identification of such a bisaddition pattern along the $C_{59}N$ cage. Interestingly, the addition of the second malonate unit upshifts the LUMO level of **(±)-3** above that of the parent $(C_{59}N)_2$ by 0.08 eV. The latter is a remarkable change on the electron accepting properties of the $C_{59}N$ cage. Despite $C_{59}N$ is the most explored heterofullerene, it lacks designing strategies towards the regioselective synthesis of bisadducts with desired electronic properties. Up to date, a mixture of $C_{59}N$-bisadducts has been evaluated in bulk heterojunction solar cells manifesting the potential for energy conversion applications.[5] The demonstrated regioselective synthesis of $C_{59}N$ bisadducts addresses the quest for molecular manipulation towards efficient fullerene-based electron acceptors. The influential benefits of this strategy could be further exploited to manipulate the band structure of heterofullerene cages by the integration of different addition patterns.



C_1, equatorial$_{face}$

Acknowledgement
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P28 - Polyacrylonitrile Based Stabilized Nanofibers and Carbon Nanofibers

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More than 90 percent of all commercial micron sized carbon fibers are produced by the thermal conversion of PAN precursor fibers. PAN-based carbon fibers are produced in three separate process steps: polymerization and wet spinning, stabilization, and carbonization.In addition to use as of polyacrylonitrile based fibers as a carbon fiber precursor, oxidized PAN fiber can also be used to produce high-performance flame-resistant (FR) materials. Carbon nanofibers(CNFs) have a potential of applications of supercapacitor, battery, and catalyst support materials. Copolymers of AN have been synthesized by free radical polymerization, and electrospun to obtain nanofibers with rotating and fixed collectors. As increase in the polymer weight percentage (PAN in DMF) resulted an increase in viscosity and nanofiber diameter where viscosity is a significant parameter for electrospinning .Acidic co-monomers itaconic acid , acrylic acid improve the hyrophilicity of the PAN precursor and catalyzes the cyclization of nitrile groups during the stabilization process by forming ladder structure.

Precursor and carbonized nanofibers were characterized by FTIR-ATR and Electrochemical impedance spectroscopy (EIS),XPS and Thermal measurements (DSC,TGA) . Fitting with equivalent circuit modelling exhibited a good correlation between the calculated and experimental values. High specific capacitance values are obtained in 0.5 M H_2SO_4 compared to 0.1 M $NaClO_4$ (Fig.1).Surface morphology of the fibers was observed by SEM and average fiber diameter was calculated through the fabrication steps. The control of nanofiber diameter and oxidation parameters is decisive for the electrical conductivity and mechanical properties of the final carbon nanofiber mats. Both inter and intramolecular reactions contribute to the observed changes in the stabilized polymer-that is, coloration, stabilization and flame resistance. High degree of homogeneity and surface induced by electrospinning improve the electrical transport properties and stability of CNFs, which are critical for high-performance organic electronics and supercapacitors

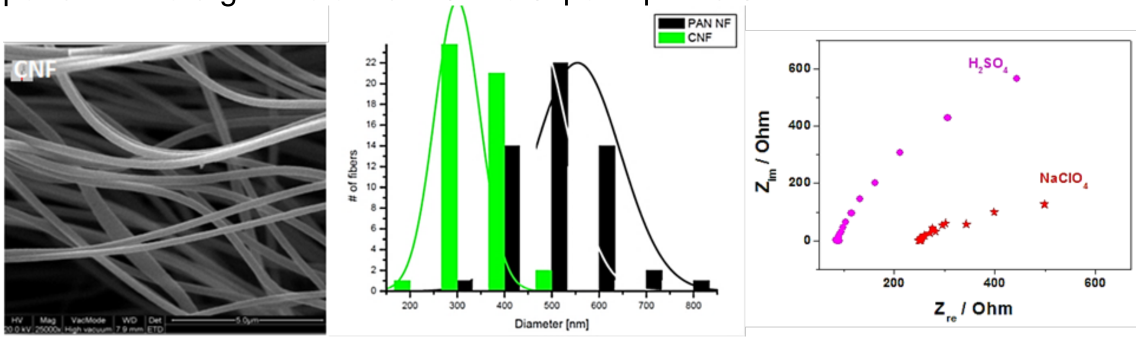

Fig1. SEM image of CNF ,PAN and CNF diameter distribution and Nyquist Plot in aq.electrolytes of CNF

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P29 - Characterization of nanocomposites based on Al-alloy and multiwall carbon nanotubes prepared by industrial High Pressure Die Casting method

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Further development of the transport industry is based on two main goals, finding of new lightweight materials with changed mechanical properties and the adoption of environmentally friendly technologies. Materials showing great potential through changed and targeted mechanical properties are nanocomposites based on a polymer matrix or metal [1,2]. Use of nanocomposites in parts production could result in a reduction of part dimensions, and eventually on a weight of a final part.

Aluminium alloys are used massively in the vehicle parts production manufacture, so the possibility for preparation of nanocomposites based on aluminum alloy AlSi9Cu3(Fe) and multiwall carbon nanotubes (MWCNTS) by the High Pressure Die Casting method (HPDC) was investigated. Nanocomposite samples were prepared on industrial HPDC machine Buhler 42D by placing MWCNTs before piston and directly in the tool with a different ratios 0.05, 0.1 and 0.2 wt. %. Degradation of MWCNTs introduced in Aluminium alloy at 690°C did not occurred that was confirmed by a scanning electron microscopy. Microstructural, metallographic and mechanical properties were studied by an optical microscope and universal testing machine. Nanocomposites with 0.05 wt.% MWCNTs placed before a piston showed finest microstructure, with smaller primary grain size of Al, that was in a correlation with the mechanical testing results, increased elongation at break and tensile strength.

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P30 - Electrospinning of ethylene vinyl acetate/ multiwall carbon nanotubes fibers

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The semicrystalline copolymer ethylene vinyl acetate (EVA) is a flexible and non-toxic polymer. EVA is an inexpensive and convenient polymer with variety of properties that highly depends on the ratio of ethylene to vinyl acetate units. Composite materials based on polymer/carbon nanotubes are interesting materials with enhanced properties compared to pure polymers. The addition of multiwall carbon nanotubes (MWCNT) can improve wide range of properties including electrical conductivity, mechanical and thermal properties. Electrospinning is now widely exploited as a versatile and straightforward method for generating ultrathin fibers made of various materials, but mostly polymer materials are used [1].

Nanocomposites based on EVA with a vinyl acetate content of 34 wt. % and various amount of MWCNT were prepared by electrospinning method. MWCNT dispersion in solution was improved by addition of compatibilizer cholesteryl 1-pyrenecarboxylate (PyChol). Results of transmission electron microscopy showed that MWCNT were aligned inside of the elastomeric matrix by process of electrospinning. The morphology of the fibers was evaluated by scanning and transmission electron microscopy. The chemical structure and composition of prepared fibres was investigated by Fourier Transform Infrared Spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) analysis. The thermal stability was tested with thermogravimetric analysis. The presence of the MWCNT inside the fibers enhanced the thermal stability of prepared nanocomposites.

Acknowledgement
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P31 - Dielectric relaxation in PDMS/TiO_2 nanocomposites

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Polydimethylsiloxane (PDMS) is an organic polymer, which is widely applied due to its optical and mechanical properties, chemical stability, easy fabrication and relatively low cost [1]. Pure PDMS is an electrical insulator at room temperature with glass transition temperature ~148 K. Combining the insulating PDMS as a composite matrix and semiconducting TiO_2 as a filler the result could lead to a material with new set of properties.

In this contribution the dielectric properties of PDMS composites containing 100 nm average size of TiO_2 particles and concentration 0 – 40 vol.% were investigated. Results revealed the increase of dielectric permittivity with increasing filler concentration and the dielectric relaxation at low temperatures, which could be related to the transition from elastic to glassy state.

In this presentation the influence of TiO_2 particle concentration on dielectric properties of PDMS/TiO_2 nanocomposites will be discussed.

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P32 - Zinc oxide – reduced graphene oxide nanocomposite dispersed in sepiolite to enhance alginate film properties

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Alginate biopolymer has good film forming capability, but the poor mechanical and barrier properties limits its application. A strategy to improve this drawback is the incorporation of inorganic materials, as zinc oxide – reduced graphene oxide (ZnO-rGO) nanofiller into the biopolymer matrix [1]. Besides that, new functionalities can be added to the film with this nanofiller, such as antimicrobial activity and electrical conductivity, respectively. However, the ZnO-rGO nanofiller has weak dispersion in aqueous polymeric matrix. To solve this problem, herein, hydrothermally synthetized ZnO-rGO filler are intercalated into fibrous sepiolite clay and added to an alginate solution in different concentrations. The bionanocomposite films are prepared by solvent casting methodology. To turn the films more resistant to water, an immersion of films in CaCl2 is done for the complexation of Ca2+ ion with the alginate. Physical and chemical characterization, such as mechanical properties, solubility and wettability were determined. The presence of zinc oxide and sepiolite in alginate films is confirmed by their typical diffraction peaks in XRD analysis. Cross-section scanning electron morphology (SEM) images of alginate films show that the use of sepiolite increase the homogenization of rGO-ZnO within alginate. Moreover, it is possible to discriminate the fibers of sepiolite and the layers of reduced graphene oxide. Electrical conductivity is also evaluated. The incorporation of ZnO-rGO filler into alginate films increase their electrical properties. The inherent properties of alginate biopolymer together with the rGO-ZnO filler allow to open doors for the application of these bionanocomposite in different fields, such as food packaging or biomedical application.

Acknowledgment:

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P33 - Wake potential in a graphene-sapphire-graphene structure

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We study the wake effect induced by an external charged particle which moves above various sy_1-Al_2O_3-sy_2 composites, where sy_i (i=1,2) may be vacuum, pristine (undoped) or doped graphene. The polarization functions of graphene sheets are obtained using two approaches within the random phase approximation [1]: an *ab initio* method and a method based on the massless Dirac fermion approximation. The dynamic response of the layer of Al_2O_3 (sapphire) is described by a dielectric function consisting of several Lorentzian terms [1]. We evaluate the total electrostatic potential in the plane of the upper graphene sheet (the wake potential). It is shown that in the low velocity limit (below a velocity threshold for the wake given by the Fermi speed of graphene) the charged particle excites only the transverse optical (TO) phonons in the Al_2O_3 slab and only those phonons contribute to the wake potential. It is also shown that the wake potential is only sensitive on the upper system sy_2 such that if sy_2 is vacuum then TO phonons give intensive oscillations which are strongly reduced if sy_2 is graphene.

Acknowledgement:
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P34 - Complex supramolecular systems *via* subcomponent self-assembly

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The use of chemical self-assembly as a synthetic technique can simplify materials preparation by shifting intellectual effort away from designing molecules, and towards the design of *chemical systems* that are capable of self-assembling in such a way as to express desired properties and functions. In Figure 1 are shown the subcomponent precursors and structures of three of products that can form functional constituents of these systems.

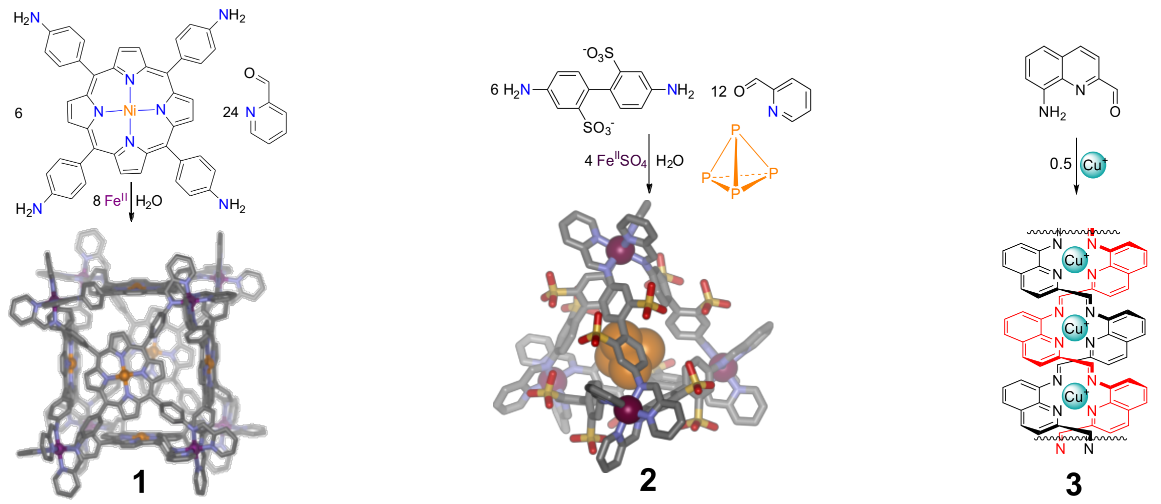

Figure 1. *Fe$^{II}_8$ cubic cage **1**,*[1] *Fe$^{II}_4$ tetrahedral cage **2**,*[2] *and electroluminescent Cu$^{I}_n$ double-helical polymer **3***[3]

Current challenges involve inducing multiple structures to form in parallel,[4] such that they may act in concert to achieve a catalytic goal.[5] Our techniques thus provide a point of entry into the emerging field of *systems chemistry*.[6] Functional systems that we have recently developed include a fuel-controlled self-assembly process[7] and a series of cages that can phase-segregate[8] and transit between liquid phases.[9] Work in progress involving the conjugation of our structures to nanocarbons will be discussed.

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P35 - Easy tools for microtexture nanoparticles tuning: exploring the flexibility of a spark generator system

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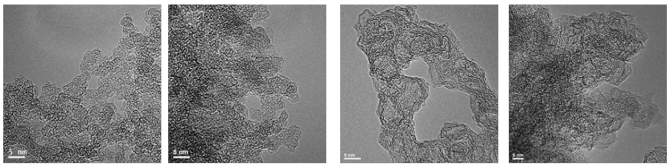
The need of easy tools for carbonaceous nanoparticles tailoring is a constant trend topic in multidisciplinary contexts, collecting a wide interest ranging from material to environmental and health research fields also in view to ensure the availability of suitable and reliable standard materials. Carbonaceous particulates generated by Spark Discharge Generators (SDGs) are produced through the vaporization of two electrodes kept at a fixed potential difference and have been widely adopted in most research studies [1] involving human inhalation and exposure to mimic carbonaceous aerosols emitted from combustion processes [2] in terms of mobility diameter and surface characteristics [1]. The SDG generated particulate is typically high-porous and nanotextured (large surface-to-volume ratio) and its production is easy-operational and allows control, reproducibility, versatility and reasonable yields (use of parallel SDGs). An important feature offered by the use of SDGs is the possibility to gain dimensionally monodisperse and high-surface purity nanoparticles [3] with an undetectable presence on the particles surface of combustion byproducts as tar-like species or polycyclic aromatic hydrocarbons. By acting on the operative parameters (rods, spark discharge frequency, dilution gases) it is possible to varying sizing, concentration of particles in the aerosol and overall chemical-physical features of the generated particulate (carbonaceous, metallic, metal-oxides or composites) [3]. In this work we pose attention to the nanotexture tuning of carbonaceous nanoparticles produced by a SDG Palas GFG 1000 type from graphite rods, by acting on three parameters: gas carrier, gas purity, discharge frequency. The chemical reactivity and the surface chemistry of the particles have been evaluated by thermogravimetry (TG) and infrared spectroscopy (FTIR) crossing the findings with the morphology and internal structural characteristics inferred by transmission electron microscopy (HRTEM). Eight samples were produced and named accordingly with gas carrier (nitrogen, argon), gas purity (99 and 99.999%, i.e. 2.0 and 5.0, respectively), discharge frequency (50, 300 Hz).



Ar 5.0, 50 Hz   Ar 5.0, 300 Hz   N2 5.0, 50 Hz N_2 5.0, 300 Hz

This preliminary survey demonstrates that tunable microtextures of carbonaceous particles are obtainable by a SDG by simply acting on the operating conditions and on the quality of gas supply. Moreover, it was found that the use of N_2 as dilution gas allows the incorporation of small quantities of N (up to 6 wt.%) in the carbonaceous particulate moiety.

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P36 - Surface attachment of Mn(III) SCO compound on FLG

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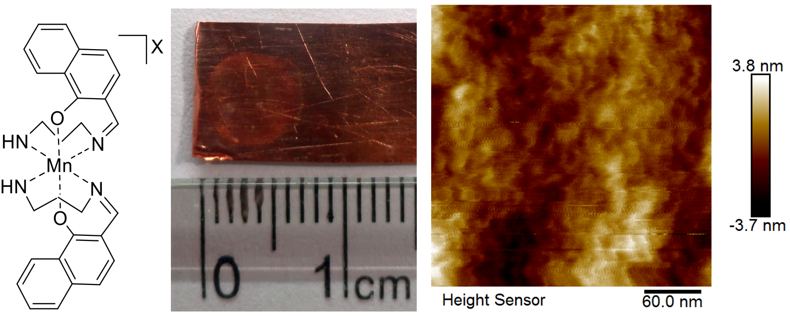
The phenomenon of spin crossover in metal complexes is known since the early 1930s,[1] and has attracted since then a lot of interest. Through their possible hysteretic effects, potential applications of these molecules include their use as molecular switches in data storage and in displays.[2–4] At low temperatures, it is energetically favorable for spin crossover compounds to be in a low spin state, and by application of an external stimulus, like heat, light, pressure or applied magnetic field,[5,6] it is possible for the spins to occupy the energetically higher orbitals, resulting in a high-spin state of the molecule.

We have synthesized a coordination Mn(III) complexes based on Schiff base with a conjugated π-system (see Figure) and have its magnetic behavior, showing the start of a spin transition. This compound weas used in combination with Few-Layered Graphene (FLG) bulk, to investigate the bond behaviour towards graphene. The bulk material was afterwards characterized by IR spectroscopy, to proof that the metal containing complex is still intact. Additionally, graphene film (CVD graphene on Cu) was used to attach a thin layer of metal complexes on the surface. The used complex contains a bulky naphthaldehyde, which is supposed to form π–π bonds between the layer and the ligand around the metal centre which allowed the synthesis of new materials. The synthesized materials were analysed by Raman Spectroscopy, AFM and high-resolution SEM.



(a) (b) (c)

Figure 1. (a) Schematic structure of Mn(III) complex with X = BPh4 (1). (b) surface attachment of the complex on to graphene coated Copper. (c) AFM image of the surface, including the hight.

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P 37 - Doping of the graphene with pt nanoparticles by pulsed laser deposition

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Pulsed laser deposition is a simple and a highly versatile technique for production of thin films. It uses the energy of a high-power pulsed laser beam to vaporize a small amount of material from a target, which is consequently deposited onto an appropriate substrate. The products obtained with this technique are thin films, which have been demonstrated as beneficial to improving the sensitivity and response time of sensing devices. Another reason why this technique is attractive for fabrication of sensors is the possibility to control the film microstructure, and hence, the properties of the films by optimizing the experimental parameters depending on the final application.

Deposition and doping of graphene films with Pt was performed by a pulsed UV excimer laser with a 193 nm wavelength, repetition rate of 10 Hz and laser beam energy of 100 mJ/pulse.

Deposited films were assayed by means of Raman and UV/Vis spectroscopy, SEM and TEM microscopy, as well as measurement of water contact angles, resistivity and sensor properties. It is considered that the produced films are good candidates for use in gas sensing applications.

Keywords: pulsed laser deposition, graphene, Pt, gas sensor, thin films.

P38 - Controlled Assembly of Graphene Networks Using Polymer Latex Crystal Templates

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Graphene has attracted enormous interest in the scientific community as the first 2D material with exceptional mechanical [1], electronic [2] and thermal [3] properties. Pristine Graphene is notoriously difficult to process for macroscale applications, to overcome this many people use graphene oxide (GO) instead. GO is water soluble and easily functionalised and so can be simply processed into various systems. GO lacks the exceptional electronic properties of graphene due to structural disorder, therefore an important area of research is on the reduction of GO, which partly restores the structure and properties of graphene. Various techniques have been developed to perform the reduction step. We report a simple approach for preparing conductive Polymer Latex-rGO composites by using a latex-assembly method [4]. After a treatment in the oven at low T, we can reduce the GO in situ. We make use of the inherent GO properties to optimise the aqueous composite fabrication, which is scalable and adaptable, and then restore conductivity with a simple, low temperature, heating step; opening up pathways to tunable electronic composite materials on a large scale.

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P39 - PLA-based multi-functional nanocomposites with improved properties for FDM 3D printing applications

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The polymer matrix used in this study was Ingeo™ Biopolymer PLA-3D850 (Nature Works) grade, developed especially for manufacturing 3D printer monofilament. Two types of carbon nanofillers were used: industrial graphene and multiwalled carbon nanotubes (TNIGNP, TNIMH4) and, respectively, those of higher quality (TNGNP and NANOCYL® NC7000 ™). Two procedures for preparing of PLA-based nanocomposites were applied using the melt mixing method by means of a twin-screw extruder: 1) Direct melt blending of the PLA polymer in the form of pellets with industrial carbon nanofillers and 2) Direct blending in the melt of the PLA in the form of powder with a higher quality carbon nanofiller. Mono-filler PLA based composites with MWCNTs obtained by the first procedure are optimal in terms of electrical conductivity around the rheological percolation threshold of 1.5 wt%. Mono-filler GNP-based composites, based on the first procedure are optimal in terms of electrical conductivity around the rheologically established percolation threshold of 6 wt%. Small synergistic effect was observed in the GNP/MWCNT/PLA bi-filler hybrid composites, when combining GNP and CNT at a ratio of 3%GNP/3%CNT and 1.5%GNP:4.5%CNT, showing higher electrical conductivity with respect to the systems incorporating individual CNTs and GNPs, at the same overall filler concentration. It was found that the mono-filler PLA-based composites with graphene obtained by first procedure, after the rheological percolation threshold of 6 wt% are optimal in terms of thermal conductivity. PLA-based composites with MWCNTs obtained by the second procedure are optimal in terms of electrical conductivity around the rheological threshold of percolation below 1 wt%. A protocol for obtaining of filament for 3D printer, using a single screw extruder, has been optimized.

Acknowledgement

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P40 - Biodegradable, elastic, electrospun polyurethane/graphene oxide scaffolds for soft tissue engineering application

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Production of scaffolds aimed for soft tissue application with sufficient mechanical properties is still a challenge. In this work, 3D porous electrospun scaffolds based on DegraPol®, a polyester urethane, with different concentrations of graphene oxide (0.0–2.0 wt%) were obtained. In order to produce scaffolds with increased porosity, solutions of DegraPol® (DP) and graphene oxide (GO) were co-electrospun with a water soluble polymer, polyethylene oxide (PEO), which was subsequently removed. Morphological and mechanical properties of the biodegradable DP and DP/GO scaffolds were analyzed and also their in vivo behavior was examined on a white laboratory rat. The electrospinning resulted in formation of porous and fibrous scaffolds with randomly oriented fibers and with mechanical properties far beyond the mechanical properties of most of the soft tissue. The co-electrospinning resulted in formation of scaffolds with higher porosity but with deteriorated mechanical properties. The results of the histological tissue analysis, performed after three months from scaffolds implantation, showed their degradation, absence of an inflammatory process and penetration of tissue cells in the scaffolds. It can be concluded that the obtained scaffolds are biodegradable, biocompatible, with optimal interconnected pore structure and with high enough porosity making them a potential material for soft tissue engineering.

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P41 - Carbon nanomaterials in removing of organic compounds from water

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Carbon nanomaterials are effective adsorbents for water treatment. The application of carbon nanomaterials in water and wastewater treatment for the removing of organic compounds has drawn wide attention. The availability of carbon-based nanoparticles does not depend on natural reserves and production can be performed in unlimited quantities as long as raw materials for synthesis are available. The unique physical and chemical properties of carbon based nanomaterials determine a wide range of options for practical applications, which in turn trigger the increase of their production. Due to their small sizes and thus large specific surface areas, nanomaterials have strong adsorption capacities and reactivity.

Keywords: carbon nanomaterials, water, organic compounds, adsorption.

P42 - Towards Graphite- and Graphene-supported Heterogeneous Ullmann Catalyst Composites

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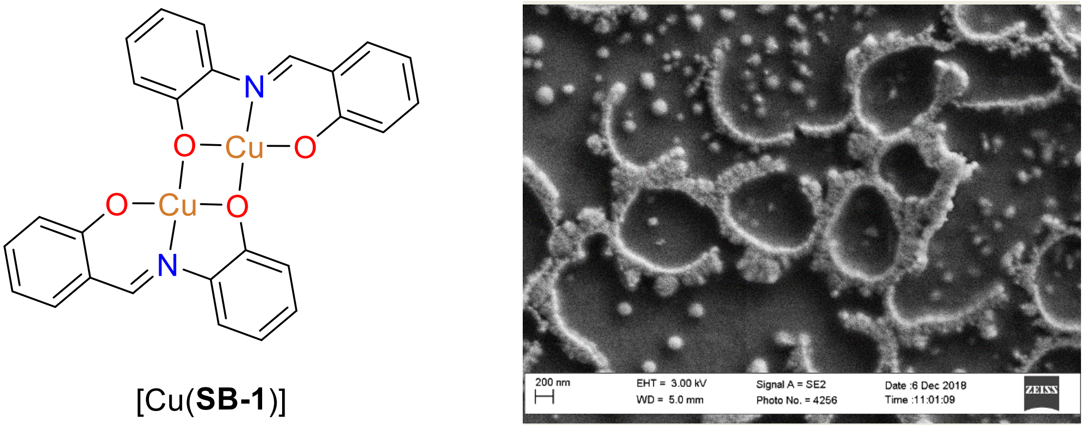
Ullmann catalysts are one of the earliest known C–C coupling agents, comprising copper in states from metallic powders to Cu(II)-ligand species, yet new variations of catalysts design and reaction conditions are continually being reported in the literature.[1] A disadvantage of ligand-based Ullmann catalysts is separation of the catalyst from the reaction mixture and often high catalyst loadings. Fixing the catalyst to a heterogeneous substrate is expected to alleviate this issue and potentially change the catalytic properties through presenting defined orientations of the complexes on a surface.

We have investigated the use of composite materials consisting of Cu(II) complexes with a simple Schiff-base, [Cu(**SB-1**)] deposited by evaporation or precipitation onto graphite or graphene substrates. [Cu(**SB-1**)] is a coordination polymer that can be dissolved into monomers and complexed with pyridine ligands,[2] resulting in a wide range of potential Ullmann catalysts. Imaging of the deposited complex on the substrates reveals differing modes of crystallisation, surface roughness and particle size as a function of deposition method.



[Cu(**SB-1**)]

Figure 1: Left: [Cu(**SB-1**)] dimer. Right: SEM of deposition of [Cu(**SB-1**)] on graphene.

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P43 - Carbon-clay nanostructured materials: application in the catalytical hydrodechlorination of chlorophenols

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Diverse carbon-clay hybrid materials showing characteristics of interest for applications in energy generation and storage, sorbents, additives in polymers and heterogeneous catalysts amongst others have been developed in the last decade [1]. Bottom-up and top-down approaches have been applied in the preparation of carbon-clay materials: from one side, graphene-like compounds can be generated from organic compounds such as polysaccharides assembled to clay substrates, and on the other side they can be obtained by direct assembly of carbonaceous materials such as multiwall carbon nanotubes (MWCNT) or graphene nanoplatelets (GNP) and clay minerals [2].

The present work refers to the top-down synthesis of carbon-clay functional materials by direct assembly in aqueous phase between GNP and the clay mineral sepiolite of rheological degree (Pangel S9, Tolsa SA). This type of sepiolite allows the formation of viscous, homogeneous and stable dispersions of GNP in water under sonomechanical treatments [3]. In addition, the presence of this silicate facilitates the incorporation of additional nanomaterials in the dispersion generating *à la carte* multifunctional materials. In this case, MWCNT and Pd nanoparticles produced from $PdCl_2$ followed by reduction using $NaBH_4$ have been also incorporated in the carbon-clay nanocomposites. These carbon-clay nanocomposites showed chemical, electrical and textural characteristics that depend on the proportion of each involved component. According to TEM images, the Pd nanoparticles exhibit a quite narrow size in all the prepared carbon-clay samples. The resulting materials have been tested in catalytic hydrodechlorination reaction (HDC) in the conversion of 4-chlorophenol (4-CPh). This process is useful to remove organic chlorinated compounds such as herbicides, pharmaceuticals, disinfection products, etc. frequently present in wastewater. The studied carbon-sepiolite/Pd nanocomposites act as very efficient and selective heterogeneous catalysts in HDC, showing in all cases exclusive selectivity towards phenol indicating that this carbon-clay systems represent a promising new approach for catalytic applications [2].

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P44 - Polymer/nanotube composites: insights from NMR studies

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Carbon nanotubes (CNTs) added to a polymer matrix strongly affect the rheological behavior that in turn may hamper the overall performance of the resulting composite. Research in this topic has focused on bulk rheological properties, while here we employ NMR diffusion experiments to explore the mobility (diffusivity) of epoxy molecules when loaded with CNTs. Rheology and light microscopy indicate percolation, or jamming events of CNT aggregates. Those aggregates cage a substantial amount of epoxy molecules while small angle X-ray scattering indicates some rearrangement of epoxy molecules in the vicinity of the nanotubes. NMR diffusion experiments distinguish between the slow diffusion of the caged molecules and that of the free ones, and relate the fraction of the former to the macroscopic system viscosity. The demonstrated surface-induced slowing-down of diffusion is both large and long-range, attributed to strong intermolecular π-π interactions between epoxy molecules and between them and the CNT surface. These findings demonstrate the utility of NMR diffusion experiments as an additional method applied to nanocomposites.

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P45 - Mechanical properties of newly formed nanomodified PMMA/AuNPs denture base material

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INTRODUCTION: This study focuses on the development and characterization of new denture base material with adequate mechanical characteristics. The mechanical properties of gold nanomodified PMMA/AuNPs and its comparation with conventional PMMA denture base material is described.

PURPOSE: Aim of the study is evaluation of some of physical and mechanical properties of heat-cured PMMA incorporated with different amounts of gold nanoparticles (AuNPs).

MATERIAL AND METHODS: In our investigation we used gold nanoparticles (GNPs) produced by new technologies - Ultrasonic Spray Pyrolysis (USP) method, from the precursor solution from Au (III). Specimens made from heat-cured PMMA containing 0.12, 0.43, 0.74 wt.% Au were evaluated. Specimens without filler served as control. The resulting nanocomposites undergo to evaluation of various physical and mechanical analysis: microhardness, dynamic mechanical analysis (DMA), flexural strength (modulus of elasticity), to evaluate their basic functional properties.

RESULTS: AuNPs-PMMA were successfully loaded and uniformly immobilized into PMMA denture base acrylic material. Modulus of elasticity decreased (PMMA-AuNP1 – 2477,90 Mpa, PMMA-AuNP3 – 2503,20 Mpa, PMMA-AuNP2 – 2657,73 Mpa) according to control group PMMA – 2703,94 Mpa). Microhardness increased from the control sample of pure PMMA to the PMMA-AuNP3 sample. PMMA-AuNP2 sample possessed the highest value of the microhardness, and the PMMA-AuNP3 sample the minimum microhardness value. DMA analysis show that the modulus of elasticity with temperature decreased linearly by all samples. The change in the modulus of elasticity can be observed at a point above 60 °C. The reference value of the modulus of elasticity was, for all samples, about 2 E + 0,9 Pa. In the area of glass transition, the modulus of elasticity dropped drastically and, therefore, the material was not suitable for use at temperatures just before and above the glass transition.

CONCLUSION: PMMA denture acrylic material loaded with AuNPs could be a possible intrinsic denture material with proper mechanical characteristics, meeting those specified for denture bases. The future researches, necessary to obtain more results including biocompatibility, color stability, agening and antimicrobial influence were still required.

KEY WORDS: Gold nanoparticles, polymethilmethacrylate, denture base, nanocomposite, mechanical properties, characterisation

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P46 - Graphene-coated textiles: a platform for wearable electronics

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We review current trends of wearable electronics and the potential of graphene-related materials within this topic. We discuss the use of graphene as material to be used as transparent electrode with examples. We then give an overview of doping graphene by surface charge transfer and show it can be used to modulate graphene's electronic properties and as a chemical sensor. We show that tunable electronic properties also have an impact on graphene biological interactions.

P47 - Freestanding electrodes based on reduced graphene oxide for supercapacitors

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The renewal of interest to fundamental mechanisms of energy storage in electrochemical supercapacitors (SCs) was boosted by the progress in development of novel (mainly carbon based) materials for nanostructured electrodes. SCs can be charged faster than batteries, leading to a very high power density, and do not lose their storage capabilities over time. The main shortcoming of SCs is their low energy density, meaning that the amount of energy, which SCs can store, per unit weight is very small, particularly when compared to batteries.

There is a wide choice of materials for the electrodes and electrolytes but all of them have limitations. Preliminary design criteria and cell specifications are following: flexible, low weight and cheap. Thus, obtaining the freestanding electrodes by simple vacuum filtration will decrease the total weight of full cell device and total cost.

Three composites based on reduced graphene oxide (rGO) were obtained in the thick film (freestanding paper) form by simple filtration with the objective to verify their possible use in supercapacitors: rGO and polycarbonate, obtained at 180°C (rGO+poly); rGO and Ni nanoparticles, obtained at 180°C (rGO+Ni_{NPS}); rGO and KCl, obtained at 700°C (rGO+KCl).

All samples were obtained by simple vacuum filtration and studied using structural (XRD, XPS), electrical (I-V) and electrochemical (cyclic voltammetry and electrochemical impedance spectroscopy) techniques. The electrochemical experiments were performed in 1M Na_2SO_4 solution purged with argon to remove dissolved O_2 with an AUTOLAB PGSTAT 302N potentiostat in a three electrode configuration.

In result, high capacitance but also high resistance were detected for the rGO+Ni_{NPs} and rGO+KCl composites. The reversible electrochemical response was obtained only for the rGO+poly. All the composites represented layered structure of freestanding paper. Among all samples rGO+poly has the highest potential for use in supercapacitors, despite that it is also very resistive. Another problem that limits their applicability is fragility. If both fragility and electrical resistance are solved these materials may be good candidates for supercapacitors.

P48 - Functionnalized CNTFETs for gas sensing

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Environmental monitoring is required to protect the public and the environment from toxic contaminants and pathogens that can be released into a variety of media including air, soil, and water. Recent advances in nanomaterials provided a strong potential to create gas sensors providing sensitivity at the single molecule level with low cost and power consumption [1]. Carbone nanotubes, are among the best promising candidate for the future development of nanosensors applications because of its high conductivity, high surface-over volume ratio and highly crystalline surface which favor gas adsorption [2]. Carbon nanotubes are very sensitive to all gases, down to very low (ppb level) concentrations [3]. However, intrinsically, carbon nanotubes based electronic devices do not prove selective to any specific gas; they rather tend to measure the variations of the global gas content. In this work, we present a new approach based on the non-covalent functionalization of the active layer of the sensor (carbon nanotubes) using Iron(III) 5, 10, 15, 30-(tetraphenyl) porphyrin chloride to improve the selectivity of the sensor. SWCNTs were synthetized by double hot filament chemical vapor deposition (d-HFCVD) on SiO_2/Si substrates. Scanning and transmission electron microscopy, Energy Dispersive X-ray (EDX) and Raman spectroscopy reveal that the Iron(III) 5, 10, 15, 30-(tetraphenyl) porphyrin chloride assembly in a non-covalent way on the surface of carbon nanotubes with extended π system. Evidence of a charge transfer between Iron and carbon nanotubes were confirmed by electrical measurements using CNTFETs .

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P49 - Graphene nanoplatelets coating for corrosion protection of aluminum substrate

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The corrosion of metal structures is recognized as one of the most serious problems in the modern societies as it results in the loss of more than one hundred billions of dollars in damage each year [1]. Intense efforts have been made to find protective coatings that inhibit the process of metal corrosion. Recently, graphene is considered as a highly promising new coating material for corrosion inhibiting coatings [2], because of its impermeability and hydrophobic properties [3,4], which allow it to create a barrier against gases and liquids when it is in a corrosive environment. The graphene is considered chemically and thermally stable [5,6], inert under different atmosphere [7], low cost coating and environmental friendly. In this work, we study the properties of graphene nanoplatelets as an effective anticorrosion coating for aluminum substrate in 0.5 M NaCl at room temperature (25°C). Scanning and transmission electron microscopy and Raman spectroscopy reveal the high quality multilayer graphene nanoplatelets. The modification of the corrosion resistance characteristic were investigated by open circuit potential (OCP), followed by electrochemical tests such as potentiodynamic polarization (Tafel curves) and electrochemical impedance spectroscopy (EIS). The electrochemical results show that the graphene nanoplatelets provides effective resistance against corrosive medium. Scanning electron microscopy (SEM), Raman spectroscopy and Energy Dispersive X-ray (EDX) studies carried after immersion in corrosive medium confirm that graphene coated aluminum surface is well protected compared to the uncoated substrate.

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P50 - Ultrafine Dispersion of Graphene Oxide Nanoplatelets in a Magnetic Iron Oxide Matrix by Heterocoagulation

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Composite dispersions of nanostructured materials containing magnetite (Fe_3O_4) nanoparticles (MNPs) and graphene oxide (GO) lamellae have been prepared by a mild and easily upscalable procedure. The charge regulated adhesion of bare MNPs to GO results in the formation of stable and uniform nanocomposite materials in a wide composition range without any preliminary functionalization steps or harsh conditions that may lead to chemical degradation of the graphene-based nanosheets [1]. Owing to the enormous surface area and negative surface charge developed in aqueous suspensions GO particles were able to accommodate MNPs that represent masses up to 50 times larger than the lamellar carbonaceous host. The macroscopic-scale observations and electron microscopy studies suggest that there is a strong interaction between the Fe_3O_4 and the GO surfaces. The oppositely charged GO and magnetite nanoparticles form huge secondary particles in the lower MNP/GO mass ratio region probably due to the bridging of GO lamellae via MNPs. Large variation in the compositions affords highly different nanostructures ranging from “house of cards” arrangement of MNP decorated exfoliated graphite oxide particles at 2/1 and 1/1 GO/MNP ratios to GO nanosheets matrixed into bulk amounts of magnetite at higher loadings. However, as the MNP/GO mass ratio further increases, the average hydrodynamic diameters of dispersed particles successively decrease reaching the submicron scale (from 2700 down to 400 nm), while the zeta potential was -30 mV for pristine GO sheets and it rose above +35 mV with increasing the MNP loading in the pH range of 4.5-6. The potential use of the magnetic nanocomposites was demonstrated by their heating efficiency for a potential future use in hyperthermic cancer therapy [2].

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P51 - Cyto- and genotoxicity of different classes of manufactured nanomaterials in alveolar epithelial cells

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The toxicological assessment of the potential toxicity of manufactured nanomaterials (MNMs) is urgently needed due to their increased use for commercial and industrial applications. Thus, this study evaluated the cyto- and genotoxicity of a panel of MNMs, including SiO_2 NPs, graphene oxide, and nano-sized pigments in rat alveolar epithelial cells (RLE-6TN), a primary target during inhalation exposure.

RLE-6TN cells were exposed for 24 h to different concentrations (0-56 μg/cm^2) of the different classes of MNMs: (1) differently capped (unmodified, phosphonate- and amino-modified), sized (7, 15 and 40 nm), and with different surface hydrophobicity SiO_2 NPs variants; (2) graphene oxide, and (3) nano-sized pigments (Cu-pthalocyanine and Cu- pthalocyanine halogenated), all dispersed in serum-free culture medium by cup horn sonication in order to evaluate their cytotoxic potential. Cytotoxicity was assessed by determining the LDH release and WST-1 metabolization in RLE-6TN cells. To evaluate the genotoxic potential of these MNMs, RLE-6TN cells were exposed to subtoxic concentrations of the different variants tested (0-28 μg/cm2) and the DNA damage was assessed by the alkaline comet assay.

Hydrophilic SiO2 NPs induced a concentration-dependent cytotoxicity in RLE-6TN cells, being the cytotoxic effect more evident in cells exposed to the smallest SiO_2 NPs. Moreover, amino and phosphonate surface modification mitigated the cytotoxicity of the unmodified SiO_2 NPs. Exposure to the hydrophobic SiO_2 NPs did not induce significant cytotoxicity on RLE-6TN cells. Graphene oxide NPs caused a concentration-dependent cytotoxicity in RLE-6TN cells. In turn, the nano-sized pigments slightly increased LDH release but failed to affect WST-1 metabolization by RLE-6TN cells. DNA damage was only observed in cells after 24 h of exposure to the two highest tested concentrations of 40 nm SiO_2 NPs.

Our data shows that the cytotoxic profile of SiO_2 NPs is influenced by the size and hydrophilic/hydrophobic nature of MNMs. In turn, amino and phosphonate surface modification attenuates cytotoxicity of SiO_2 NPs on RLE-6TN and might constitute a strategy to increase biocompatibility of SiO_2 NPs. Graphene oxide NPs were the most cytotoxic among the MNMs tested. Nevertheless, further research must be conducted to support these findings.

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P52 - Soft graphene nanocomposites for mechanical sensing and energy harvesting applications

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High permittivity and electromechanical coupling are critical to perform energy storage or conversion between mechanical and electrical energy for various applications of electrostrictive polymers. We report a giant electrostriction effect in liquid crystalline graphene doped elastomers [1]. The materials are formulated by an original phase transfer method which allows the solubilization of graphene oxide monolayers in non-polar solvents. It is shown in particular that liquid crystal transition leads to an increased percolation threshold. Because of their liquid crystal structure, the resultant composites show a giant electrostriction coefficient ($M{\sim}10^{-14}$ m^2/V^2 at 0.1 Hz) along with good reproducibility during cycles at high deformation rates. This work offers a promising pathway to design novel high performance soft dielectric materials for sensing or energy harvesting applications.

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