FCT Relatório Científico 2009 Print: 28-03-2010 23:10:43 [Centro de Química - Vila Real]

General Information

Name of Research Unit:	(QUI-Norte-616) Centro de Química - Vila Real
Coordinator:	Pedro Manuel de Melo Bandeira Tavares
Main Scientific Domain:	Química
Other Subdomains:	n/a

Host Institutions

Leading Host Institution:	Universidade de Trás-os-Montes e Alto Douro
Other Institutions Involved:	

Objectives & Achievements

Unit Description

The "Centro de Química-Vila Real" (CQVR) is a research unit of the Universidade de Trás-os-Montes e Alto Douro (UTAD). The great majority of members belong to the academic staff of the Chemistry Department of UTAD, although it also includes some researchers from Geology, Soils and Engineering Departments that share similar scientific interests. Since its creation the Unit has had a slowly but consistent growing in members. In 2009 the CQVR has 24 PhD full members with an increase to 28 PhD full members (and 1 PhD collaborator) in 2010.

The CQVR mission is to perform scientifically recognized research in areas involving Chemistry, to explore potential applications, to assist national and local industries and to contribute to the training of young researchers. Main objectives of the CQVR are to publish national and international patents in particular the ones with industrial application, good quality scientific articles in high impact factor journals and promote the formation of young researchers through MSc and PhD programs. In the last evaluation (2003-2007 period) we obtained the classification "Very Good".

In 2009 the CQVR unit was organized in three research groups that developed fundamental and applied chemistry research in the areas of Organic Chemistry, Natural Products and Food Chemistry (9 PhDs), Materials Chemistry (8 PhDs) and Environmental Chemistry (7 PhDs).

The organization of the Unit includes:

A Direction with a director and two vice-directors;

Three Principal Investigators (PI), one for each research group;

An advising committee (Direction + PI) to prepare proposals to the Scientific Committee;

A Scientific Committee that includes all the PhD members;

An International Advising committee.

The research activities of the unit have been supported mainly through national and international projects from R&D funding agencies, projects with enterprise partners, and regular FCT budget to CQVR.

The web page of CQVR Unit can be seen at: http://home.utad.pt/~cqvr/

General Objectives

This unit has 8 general objectives:

1. to perform fundamental and technological research on relevant topics involving Chemistry;

2. to provide a modern and high level of scientific training to researchers;

3. to stimulate interdisciplinary collaboration and interaction among the research groups, and with research units in other scientific areas;

4. to promote the internationalisation of the Unit;

5. to disseminate knowledge to the general public;

6. to stimulate the interest of young students in Chemistry;

7. to increase collaboration and interaction with industry;

8. to benefit the Region by putting at the service of its population and local authorities scientific knowledge and equipment.

To accomplish these objectives the following strategy has been applied:

To enhance the registration of patents and to encourage collaborative projects with companies in order to transfer knowledge created in the unit;

To publish research results in high impact peer-review journals included in the SCI;

To provided the conditions (financial, laboratorial and scientific) for the graduation of young researchers;

To provide the laboratories with modern research equipment and to promote the utilisation of this equipment to the general scientific community and enterprises;

To create additional national and international scientific collaboration with other research units, in order to overcome some of the unit difficulties, in particular those related to the lack of sophisticated, high priced equipment;

To organize scientific national and international meetings and special conferences designed to the general public;

To promote seminars of current work between the Unit members and young researchers; to invite specialists to visit the Unit and give seminars;

To participate in national programs for the hiring of young researchers, BII, BI and pós-doc.

The following main scientific topics are studied:

1. Organic Chemistry, Natural Products and Food Chemistry:

Objectives & Achievements

- Synthesis and structural characterization of organic compounds with applications in photochromic devices, photodynamic therapy, affinity chromatography and pharmaceutics.

- Structural characterization of new natural products isolated from plants and foods.

- Functional and Biological Activities of Polysaccharides and Phenolic Compounds from foods.

2. Materials Chemistry:

- Synthesis and characterization of ceramic, intermetallics and hybrid organic/inorganic materials with applications in sensors, electronic devices, magneto-cooling, optics, catalysts and solid state electrochemistry.

- Synthesis and characterization of palladium-based membranes to be used as anodes and cathodes in fuel cells.

- Synthesis of new metal complexes covalent anchored on the surface of inorganic materials to be used as hybrid organic – inorganic catalysts.

- Synthesis of materials by alkaline activation and their characterization.

3. Environmental Chemistry:

- Advanced Oxidation Processes (AOP) that can reduce the pollutant load of water and wastewaters.

- Metal-natural substrates interactions to understand the behaviour, bioavailability and ultimate fate of pollutants in the environment.

- Mineralization-Sequestration of Carbon, Nitrogen and Phosphorus: Cycling and Modelling

- Influence of groundwater pollution on geochemical processes.

- Treatment, recovery and valorisation of industrial, agricultural and agro-industrial by-products and wastes under an industrial ecologic approach.

Main Achievements during the year of 2009

The quality of the research conducted at CQVR is mainly reflected in the patents and SCI papers in high impact factor journals. Recent CQVR patents are now under industrial implementation and new contracts with industry are foreseen in a near future. Some of the CQVR papers are among the most cited ones of the UTAD and we have been invited to write review papers in top SCI journals like Advanced Materials. Many of the CQVR members are often asked to referee submitted papers.

A strong cooperation with other national and international research units is a constant allowing to full optimisation of our resources in equipment, in particularly the one acquired by the "National re-equipment project" (XRD, TGA, GC-MS, IC, HPLC). On the other hand some of our difficulties are overcome with these collaborations leading to a full cooperation. The full integration of the UTAD Microscopic Laboratory Unit (UME) in the National Electronic Microscopy Network (RNME) allows to maximize our equipment operation and to have access to top microscopy equipment.

1. The equipment acquired in the national FCT re-equipment Program: projects REEQ/1183/CTM/2005 (170.000 €) and REEQ/329/QUI/2005 (200.997€) are fully operational and available to researchers from CQVR, from other UTAD Units and from other institutions. Master and PhD students and BII's are among the top users of that equipment.

2. The FCT program "Ciência 2008" was a priority for the CQVR. We ask for 2 positions (10%) but unfortunately we obtained only 1 position from FCT (Organic Chemistry group).

3. The scientific production of this unit during the last four years was maintained and the objective of publishing in high impact SCI journals (IF>2) was successfully achieved. In 2009 we have published 4 patents (and submitted 4), 35 papers in SCI peer-review journals, 1 book, 1 book chapter and 29 conference proceedings.

4. This performance was possible due to the dynamism of the team. In 2009 we obtained approval in 5 new FCT projects that will start in 2010.

5. As always, particular attention was paid to collaboration/interaction with industry. Research protocols were continued with Águas de Trás-os-Montes e Alto Douro (ATMAD, including co-funding of a PhD grant concluded in 2009). The Licence agreement established with Cooperativa Agrícola dos Olivicultores de Murça - CAOM (regional cluster company of olive oil production) on the use of patent (PT 103 470, 2006) in project Biocombus is in progress.

Extension activities, concerning water and wastewater analysis for local councils and other public bodies were continued.

6. An International Congress (Hyceltec) was organized by CQVR members with 130 participants.

7. Diffusion was accomplished through regular scientific seminars, presentations in High Schools, Scientific Forums and Chemistry Olympics. The Centre Web page was regularly updated.

8. A great effort was made in order to improve research potential resulting in 2 PhD degrees and 10 Masters.

Activities

Integrative/multidisciplinary activities during the year of 2009

Much of the chemical research involves collaboration with other research areas such as biology, veterinary science, agronomy, geology, physics and engineering.

Two different situations can be identified:

1) Analyses, synthesis and interpretation tasks carried out by others institutions in the framework of common research projects:

- Photochemical, photokinetic and photocitotoxicity studies on new functional dyes synthesized in CQVR were made in collaboration with pharmaceutic, physics and photophysics experts of national Universities (Aveiro, Coimbra, Minho, Beira Interior, IST) and foreign Universities (Lille, Marseille, Paris VII, Toulouse, Katholieke Universiteit of Leuven).

- The biological activities of natural metabolites and the potential of functional dyes as non-covalent probes for proteins were evaluated together with the Biology Dep. of the Univ. of Minho, CECAV (UTAD) and Institute of Molecular Biology and Genetics (Ukraine).

- The complementary biological treatment of wastewaters was developed in collaboration with Dep's. of Biological and Environmental Engineering and Agronomy (UTAD). The treatment and recovery of industrial wastes was carried out in collaboration with the Environmental and Economy group of the Univ. of Aveiro and a technological innovation institute (IDITE-Minho).

- Thin film depositions (sputtering and laser ablation) were done in collaboration with INESC-Porto and CICECO - Aveiro Univ.

- Assembly/performance of LEDS were done in collaboration with Chemical and Biological Eng. of IST and Telecommunications Institute of Lisbon.

- Materials characterisations were done in collaboration with: Physics Dep. of the Oporto Univ. and Aveiro Univ. (CICECO) (electric, dielectric, magnetization, Raman, IR, Photoluminescence, Solid state 1H, 13C and 29Si NMR, FEG/SEM, AFM); Applied Physics Dep. of the Chalmers Univ. of

Activities

Technology (Göteborg, Sweden) (FTIR and FT-Raman); ISOLDE/CERN and ITN (Hyperfine techniques - PAC); Physics Dep. and Chem. Inst. of UNESP (Brazil) (SAXS).

2) Analyses, synthesis and interpretation tasks carried out by CQVR in the framework of common research projects or as services to the scientific community and industries:

- Collaboration with the Dep.s of Agronomy (antioxidant activity of chestnut varieties), Animal Science (determination of lignin and cellwall polysaccharides in animal feeds) and Veterinary Dep. (development of a method of selenium determination in diverse body tissue and environmental matrices). Analysis of fatty acids, phenolic compounds and sugars in honey, wine and food products are also being performed with diverse UTAD Dep.s.

- CQVR is involved in specific SEM/ESEM/EDS, TEM and XRD characterisations: Nanoparticles characterization (in particular the catalyst groups of FEUP and FCUP); Mineral and biological samples characterization, Geology Dep., Environmental and Biological Eng. Dep. and Veterinary Dep. of UTAD; Intermetallics, CICECO (Aveiro Univ) and IFIMUP (Oporto Univ).; Polymeric materials, Polymer Eng. Dep. of Minho Univ.

Routine analysis in AAS, GF-AAS, FTIR, DSC, TGA are performed to Eng. Dep. (Civil, Mechanics), Geology, Soils of UTAD and Physics Dep. of Aveiro Univ.

Outreach activities during the year of 2009

The CQVR has widened its approach to scientific research to the society. The Unit's aims are to reveal its activities, benefit the cultural development and to stimulate the interest of young students – the future Portuguese scientists – in Chemistry. The CQVR members were invited to give lectures on National and abroad Universities. The CQVR laboratories were visited by students from Secondary Schools from the North of Portugal.

We want to emphasise the "5th Olimpiadas de Química Júnior" (2009) with 14 schools, 45 teams, 130 students from 8th and 9th years. This is a national chemistry contest (promoted by the Portuguese Chemical Society) with questions based on the execution and observation of laboratory experiments and general chemistry knowledge.

A CQVR member of the Environmental group had participated in a television program about their research activities with broadcast on national TV (see the film in http://home.utad.pt/~cqvr/J_Claro_SICN2009.wmv)

II Curso de Actualização de Professores de 1º CEB, 1-4 Julho 2009. Practical Classes of Chemistry: M. Cristina OLIVEIRA.

"A Experimentação em Ciências Físico-Químicas":

1) Desenvolvimento dos Programas dos 7º, 8º e 9º anos da Componente de Química da disciplina de Físico-Química;

2) Desenvolvimento dos Programas dos 10º e 11º anos da Componente de Química da disciplina de Química.

Acções de Formação integradas no Centro de Formação da Associação de Escolas de Vila Real dirigidas a professores do 3º ciclo e ensino secundário.

(Workshops: 2 x 50 hours). (2/9 – 12/12/2009)

Institutions: UTAD, QREN, POPH.

J.A. PERES, M. M. OLIVEIRA (Coordinators);

CARVALHO M. J., CLARO J., DE ZEA BERMUDEZ V., FERREIRA M., NUNES F., OLIVEIRA C., REGO R., REIS. L., SANTOS P., SOUSA J., TAVARES P.B.

V. DE ZEA BERMUDEZ, "Self-assembly: a Bet in the Future", Seminars of the Dep. of Applied Chemistry of Waseda University, Tokyo (Japão), 27/5/2009

J.A. PERES, "Tratamento de Águas: aplicações ambientais ao serviço da saúde pública", STG'09 - Semana da Tecnologia e da Gestão, Escola Superior de Tecnologia e Gestão, Instituto Politécnico de Bragança, Bragança, 21/4/2009.

J.A. PERES, "Poluição de Água: novos problemas, novos desafios", IV Jornadas do Ambiente – Câmara Municipal de Vila Pouca de Aguiar, Auditório da Escola Secundária, Vila Pouca de Aguiar, 19/6/2009.

P. B. TAVARES, "Why and when using near atmospheric ESEM mode? Biological and non-biological samples", One day course on High Resolution Imaging Techniques", RNME, Universidade de Aveiro, 28/3/2009

Funding

	2008	**2009**						
LA FCT	0,00	0,00	0,00	0,00				
Units FCT	0,00	0,00	0,00	80.000,00	0,00	0,00	0,00	90.749,00
Projects FCT	0,00	0,00	0,00	48.073,00	0,00	0,00	0,00	119.403,00
Other (National)	0,00	0,00	0,00	0,00	0,00	0,00	0,00	10.600,00
Other (International)	0,00	0,00	0,00	0,00	0,00	0,00	0,00	137.144,00
National Industry	0,00	0,00	0,00	415.525,00	0,00	0,00	0,00	415.525,00
International Industry	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
	543.598,00	**773.421,00**						

General Indicators

	2005	**2006**	**2007**	**2008**	**2009**	**Total**
No. of Researchers Proposed	0,00	0,00	0,00	0,00	0,00	0,00

General Indicators

	2005	2006	2007	2008	2009	Total
No. of Researchers Hired (LA)	0,00	0,00	0,00	0,00	0,00	0,00
Balance	0,00	0,00	0,00	0,00	0,00	0,00
No. of Researchers Hired (Ciência Programme)	0,00	0,00	0,00	2,00	1,00	3,00
No. of Researchers (FTE)	16,00	16,00	20,00	23,00	23,00	
Training Masters (Master thesis completed)	3,00	2,00	1,00	3,00	10,00	19,00
Training PhDs (PhD thesis completed)	1,00	0,00	2,00	2,00	2,00	7,00

Researchers Hired

Name	Start Date	End Date	Other Institution
Dr. Prostota Yaroslav	01-07-2009	30-06-2014	

Technical Personnel Hired

Name	Start Date	End Date	Other Institution
No technical personnel found...			

Additional Comments

Research Groups

Reference	Title / Principal Investigator
RG-Norte-616-440	Materials Chemistry (Verónica Cortés de Zea Bermudez)
RG-Norte-616-1508	Organic Chemistry, Natural Products and Food Chemistry (Luis Herculano Melo de Carvalho)
RG-Norte-616-1509	Environmental Chemistry (Jose Alcides Silvestre Peres)

FCT Relatório Científico 2009 Print: 28-03-2010 23:14:23 [Centro de Química - Vila Real]

Group Description

Title of Research Group:	(RG-Norte-616-1508) Organic Chemistry, Natural Products and Food Chemistry
Principal Investigator:	Luis Herculano Melo de Carvalho
Main Scientific Domain:	Química
Group Host Institution:	Universidade de Trás-os-Montes e Alto Douro

Funding, source, dates

Funding, source, dates

Development of a new class of Photochromic Naphthopyrans, FCT- PTDC/QUI/66012/2006, PI: Paulo Coelho (CQVR), Luís Carvalho (CQVR), Maria Manuel Oliveira (CQVR), CQVR amount: 94 743 €, (2009-2011)

Thienylpyrroles as building blocks on the synthesis of organic and coordination compounds with nonlinear optical (NLO) applications, FCT-PTDC/QUI/66251/2006, PI: M.M. Raposo (U. Minho), UTAD: Paulo Coelho, Luis Carvalho, Total amount: 159 486 €, CQVR amount: 8 000 €, (2009-2011)

Fotoquímica de Superfícies: Aplicação da Fotocatálise Solar a Estudos de Descontaminação Ambiental em meios Heterogéneos, FCT- PTDC/QUI /65510/2006, PI: A. S. Oliveira (IST/UTL)

UTAD: Paulo Santos, Lucinda Reis, CQVR amount: 14 066 €, (10/3/2008 - 9/3/2011)

Fototoquímica de Superfícies: Fotoquímica e Fotofísica de Corantes Funcionais no Infravermelho Próximo em Superfícies e Nanocavidades, FCT-PTDC/QUI/70153/2006, PI: A. S. Oliveira (IST/UTL), UTAD: Paulo Santos, Lucinda Reis, CQVR amount: 11 580 (5/2/2009 - 4/2/2012)

Objectives & Achievements

Objectives

1. Synthesis and structural characterization of organic compounds with applications in photochromic devices and pharmaceutics.

2. Synthesis and structural characterization of new 2H-chromenes with fused aromatic rings.

3. Determination of photochromic properties under continuous UV irradiation conditions. Study of structure/photochromic properties relationships.

4. Determination of the kinetic and thermodynamic parameters associated to the photochromic phenomena.

5. Mechanistic studies of particular photochromic processes, including the determination of the number, structure and concentration of the thermally unstable photoisomers formed upon UV irradiation through 1H, 13C and 19F-NMR spectroscopies.

6. Mechanistic studies of photochromic compounds by electrospray tandem mass spectrometry: study of the influence of the heteroatom in fragmentation mechanisms.

7. Mechanistic studies of photochromic compounds by electrospray tandem mass spectrometry - study of the influence in fragmentation mechanisms of the following factors: annelation of the pyran ring (5,6 or 7,8) and position of substituents at the naphtho ring and/or at the sp3 carbon.

8. Synthesis of functional dyes (mainly of the squarylium and croconylium type) as sensitizers for Antimicrobial Photodynamic Therapy, as fluorescent near-infrared probes for biomolecules and as pseudo-affinity ligands for Affinity Chromatography.

9. Isolation and characterization of mushrooms polysaccharides. Evaluation of their antitumor activity.

10. Study of compounds responsible for the antioxidant activity of mushrooms.

11. Study of the antioxidant activity and phenolic compound profile of Portuguese olive oil varieties.

12. Evaluation of allelopathic activities using an in vitro culture plant model of propolis from Azores and also evaluation of the in vitro antioxidant and antimicrobial activity of different extracts of other portuguese propolis (Leiria, Vila Real and Vila Nova de Cerveira).

13. Study of lipid profile changes in brain mitochondria isolated from mouse 3xTg-AD, a model to Alzheimer`s Disease.

14. Farmacological and kinetic evaluation of tacrine derivatives.

Main Achievements

New 4-(2',2'-diphenylethenyl)naphthopyrans were synthesised and their photochromic behaviour in solution were studied. Although only one coloured photoproduct was expected to be formed, NMR analysis on degassed UV-irradiated solutions, performed at low temperature, showed the formation of different compounds. Among them, the main product is formed through a [2+2] cyclisation reaction and show thermally reversible photochromic properties.

New p-fluoro-substituted indeno-fused 3,3-diphenyl-3H-naphtho[2,1-b]pyrans were prepared and their photochromic properties studied by UV–vis and NMR spectroscopy. At room temperature UV irradiation of of one of this compounds gave rise to two diastereoisomeric TT open forms that possess an helical structure with the conjugated 3,3-diaryl-1,3-propdienyl chain out of the plane of the indeno-naphthalen-2(1H)-one core, which renders the thermal bleaching very difficult and thus increases the life-time and concentration of these coloured species.

The photochromic properties of hybrid organic-inorganic ureasilicate sol-gel films dopped with benzo- and naphthopyrans were studied. The films were transparent and flexible and for naphthopyrans they were colourless or presented just a slight colouration. Under UV continuous irradiation the films developed a significant absorption in the visible region that fades in the dark with variable kinetics depending on the naphthopyran structure. 2,2-Diphenyl-3H-naphtho[2,1-b]pyran films showed a very fast colouration under UV light giving rise to coloured open forms that practically returned to the initial absorbance in one minute.

Positive mode electrospray tandem mass spectrometry (ESI-MS/MS) could be a very useful technique for the structural characterization of the main

Objectives & Achievements

photoproducts of 2H-chromenes derived from carbazoles and that fragmentation could occur either from the CF form or the TC and/or TT forms. Information about mass spectrometric fragmentation of photochromic compounds, such as benzo- and naphthopyrans, is very scarce and all the studies were based on electron impact mass spectrometry (EI) of simple 2H-pyrans and 2H-[1]-benzopyrans being the benzopyrilium ion identified as the major fragment. In a recent work we have found differences in the fragmentation mechanism of carbazole, dibenzofuran and dibenzothiophene derivatives with the same annelation and relative position of oxygen atom of the pyran ring. Our results suggest the involvement of the allenyl-naphthol intermediate on the photochromic mechanism what makes electrospray tandem mass spectrometry a valuable tool for the study of the photochromic mechanisms of 2H-chromenes.

In the evaluation of biological properties of 4-aryl-4H-chromenes we have determined the TEAC values for all the compounds synthesized. The toxicity of the best antioxidant compounds was evaluated using mitochondria as a model.

New delocalized cationic azo dyes incorporating a bathochromic thiazole and displaying absorption close or in the near infrared have been synthesised and their solvatochromic behaviour studied

.

A new methodology to the synthesis of azobenzothioazole dyes, especially to those bearing electron withdrawing groups at the coupling component or to orto and meta substituted ones, was developed based on the condensation of 2-nitrosobenzothiazoles with an aromatic amine, for which a strong electron donating capability is dispensable.

Several squarine cyanine dyes were studied as possible fluorescent probes for the detection of proteins, particularly albumins, the majority of which shown significant fluorescent response to human serum albumin (HSA) and bovine serum albumin (BSA).

Apart from its pharmaceutical applications, propolis seems to have a great potential in agro-chemical investigation: as a source of new bioherbicides due to its strong inhibitory effect on early root development, cell proliferation and morphogenic developmental pathways, but also as a source of plant protective compounds against abiotic stress (namely high light stress) due to its stimulatory effect on chlorophyll content and protective effect of PSII activity.

Group Productivity

Publications in peer review Journals

ANA REIS, M. ROSÁRIO M. DOMINGUES, M. MANUEL OLIVEIRA, PEDRO DOMINGUES (2009) - Identification of free radicals by spin trapping with DEPMPO and MCPIO using tandem mass spectrometry, European Journal of Mass Spectrometry., 15 (6), 689-703. (IF= 1.167)

BARROS, Ana; NUNES, Fernando; BARROS, C; SILVA, A; DOMINGUES, M. (2009) - Structural characterization of nitrated 2'-hydroxychalcones by electrospray ionization tandem mass spectrometry, European Journal of Mass Spectrometry, 15, 605-616. (IF= 1.167)

BARROS, Ana; SILVA, Artur (2009) - Synthesis and structure elucidation of three series of nitro-2-styrylchromones using 1D and 2D NMR spectroscopy, Magnetic Resonance in Chemistry, 47, 885-896. (IF= 1.443)

BERTHET, Jerome, COELHO, Paulo, CARVALHO, Luis, VERMEERSCH, Gaston, DELBAERE, Stephanie (2009) "NMR investigation of the dyes formed under UV irradiation of some photochromic indeno-fused naphthopyrans". Journal of Photochemistry and Photobiology A: Chemistry, 208, 180–185 (IF= 2.362)

COELHO, Paulo, CARVALHO, Luís, MOURA, João, RAPOSO, Maria (2009) "Novel photochromic 2,2'-bithiophene azo dyes". Dyes and Pigments, 82, 130-133. (IF= 2.507)

COELHO, Paulo, CARVALHO, Luís, VERMEERSCH, Gaston, DELBAERE, Stephanie (2009) "Thermally reversible photochromic behaviour of new naphthopyrans involving a [2+2] cycloaddition reaction". Tetrahedron, 65, 5369-5376. (IF= 2.897)

DINIS, Maria; BEZERRA, Rui; NUNES, Fernando; DIAS, Albino; GUEDES, Cristina; FERREIRA, Luís; CONE, John; MARQUES, Guilhermina; BARROS, Ana; RODRIGUES, Miguel (2009) - Modification of wheat straw lignin by solid state fermentation with white-rot fungi. Bioresource Technology 100(20): 4829-4835. (IF= 4.453)

DIOGO, Cátia V., FÉLIX, Luís, VILELA, Sérgio, BURGEIRO, Ana, BARBOSA, Inês A., CARVALHO, Maria J. M., OLIVEIRA, Paulo J., PEIXOTO, Francisco P. (2009) "Mitochondrial toxicity of the natural molecules daphnetoxin and daphnoretin". Toxicology In Vitro, 23: 772–779. (IF= 2.473)

FAUSTINO, Hélio, BRANNIGAN, C. R., REIS, Lucinda V., SANTOS, Paulo F., ALMEIDA, Paulo. (2009) "Novel azobenzothiazole dyes from 2-nitrosobenzothiazoles". Dyes and Pigments, 83: 88-94. (IF= 2.507)

REIS,, Lucinda V., SERRANO, João P., ALMEIDA, Paulo, SANTOS, Paulo F. (2009) "The synthesis and characterization of novel, aza-substituted squarylium cyanine dyes". Dyes and Pigments, 81, 197-202. (IF= 2.507)

SALVADOR, Maria A., ALMEIDA, Paulo, REIS, Lucinda V., SANTOS, Paulo F. (2009) "Near-infrared absorbing delocalized cationic azo dyes". Dyes and Pigments, 83: 118–123. (IF= 2.507)

SIMÕES, J; MADUREIRA, P; NUNES, Fernando; DOMINGUES, M; VILANOVA, M; COIMBRA, M. (2009) - Immunostimulatory Properties of Coffee Mannans. Molecular Nutrition and Food Research, 53, 1036-1043. (IF= 3.308)

Other publications International

LEAL F., RODRIGUES A., FERNANDES D., NUNES F. M., CIPRIANO J., RAMOS J., TEIXEIRA S., VIEIRA S., CARVALHO L. M., PINTO-CARNIDE O. (2009) "In vitro multiplication of Calendula arvensis for secondary metabolites extraction", Acta Horticulturae (ISHS) 812, 251-256.

Coimbra AM, Fontainhas-Fernandes A, Oliveira MM, Carrola J, Peixoto F., "Histopathology and oxidative stress in barbel (Barbus bocagei) of the Vizela River (North Portugal), a first approach", Annual Meeting of the Society-for-Experimental-Biology, Comparative Biochemistry & Physiology A-Molecular & Integrative Physiology, Glasgow, Scotland, 2009, Volume: 153A, Issue: 2 Pages: S61-S62,

Other publications National

Group Productivity

Book

BARROS Ana; NUNES, Fernando; MAIA; Miguel (2009) - Manual de Boas Práticas na Produção de Cera de Abelha. Federação Nacional de Apicultura, ISBN: N/a

Master and Ph.D. thesis completed

Master thesis:

CANDIDA BARROS, "Modification of wheat straw lignin by solid state fermentation with white-rot fungi", MSc in Engenharia Zootecnia, Supervised by LUÍS FERREIRA and FERNANDO NUNES, UTAD (2009)

LUÍS MANUEL LOURENÇO FÉLIX, "Avaliação da actividade protectora do carvedilol na nefropatia". MSc in Análises Laboratoriais. Supervised by F. P. PEIXOTO and M.M. OLIVEIRA (2009).

MARIA DO CÉU SOUSA E SILVA, "Efeito do óleo extraído do café nas funções hepáticas, bioenergética mitocondrial e stresse oxidativo". MSc in Análises Laboratoriais. Supervised by M. M. OLIVEIRA AND F. P. PEIXOTO F.P, (2009).

Patents/propotypes

BARROS, Ana, NUNES, Fernando, FRAGA, Sara. Processo de obtenção de fibra dietética de cogumelos e respectiva fibra. Pedido de Patente Nacional nº104691, Ref. 40494/2009, 28/7/2009:

Organization of conferences

I Ciclo de Colóquios em Ciência Alimentar e Saúde, UTAD, 24/4/2009 and 16/6/2009, Ana Barros (CQVR)

Celebração do Dia Mundial da Alimentação (In)Segurança Alimentar, UTAD, 16/10/2009, Ana Barros(CQVR)

II Jornadas de Bioquímica da UTAD, 22-23/5/2009, M.M Oliveira (CQVR)

Mini-Fórum Ciência Viva, UTAD, November 2009, M.J. Carvalho (CQVR)

Industry contract research

Estudo das Ceras de Abelhas Nacionais, IFAP (inserido no Plano Apícola Nacional), CQVR: Ana Barros, Fernando Nunes. CQVR: 50 000 €, (2010-2012)

Internationalization

The Organic chemistry group develops its research in collaboration with other researchers of national and international research Units as can be seen by the co-authors of some of the publications:

- G Vermeersch, Jérôme Berthet and Stéphanie Delbaere (Université de Lille 2, France)

- Sergiy M. Yarmoluk and co-workers (Institute of Molecular Biology and Genetics;

- National Academy of Sciences of Ukraine;

- Daniel Lynch (Exilica Limited, UK).

Future Research

Objectives

- Synthesis of new photochromic oxazolines and naphthopyrans

We will continue our studies on photochromic molecules with the following aims:

- Development of new compounds with enhanced properties, in particular in the naphthopyran, heteroaromatic azo and oxazine families;

- Synthesis of new thermally reversible photochromic molecules with thermal stability and photoswitch properties;

- Preparation of new materials by incorporation of photochromic molecules in sol-gel matrices;

- Synthesis of new squaraine cyanine dyes in order to achieve improved fluorescent near-infrared probes for the detection and quantification of proteins.

- Synthesis of new squarylium and croconylium cyanine dyes for the development of potential sensitizers for Photodynamic Therapy (PDT), with special emphasis on Antimicrobial PDT.

- Isolation and characterization of mushrooms polysaccharides. Evaluation of their antitumor activity.

- Use of the "in bean" coffee model to study the mechanism of melanoidin formation during coffee roasting

- Study of compounds responsible for the antioxidant activity of mushrooms.

- Study of the antioxidant activity and phenolic compound profile of Portuguese olive oil varieties.

- Synthesis of phenolic derivatized chitosan polysaccharides with different acetylation degrees and molecular weights for application in fruit juice clarification.

- Preparative HPLC evaluation of different extracts of several propolis samples in order to identify and isolate their major components which will be tested in several in vitro assays. We also intend to evaluate the anti-inflammatory activity of propolis extracts.

Funding, source, dates

Future Research

Development of a new class of Photochromic Naphthopyrans, FCT- PTDC/QUI/66012/2006

PI: Paulo Coelho, L. Carvalho, M. M. Oliveira, CQVR: 94 743 €, (2009-2011)

Thienylpyrroles as building blocks on the synthesis of organic and coordination compounds with nonlinear optical (NLO) applications, FCT-PTDC/QUI /66251/2006, P. Coelho, L. Carvalho

CQVR: 8 000 €, (2009-2011)

Interacções de Afinidade entre Cianinas e Biomoléculas em Processos Cromatográficos, FCT-PTDC/QUI-QUI/100896/2008, PI: P. Almeida (UBI), UTAD: P. Santos, L. V. Reis

CQVR: 54 624 €, (2010-2012)

Estudo das Ceras de Abelhas Nacionais, IFAP (inserido no Plano Apícola Nacional), CQVR: A. Barros, F. Nunes. CQVR: 50 000 €, (2010-2012).

Projecto QREN – FITAQUA, CQVR: F. Nunes, A. Barros, M.M. Oliveira 220 000 € (2010-2012)

Pending

Design, synthesis and functional characterization of new photochromic benzo[1,3]oxazines, FCT-PTDC/QUI-BIQ/110247/2009, CQVR: P. Coelho, L. Carvalho, Y. Prostota, 117 456 €

Desenvolvimento de Corantes Esquarílicos para Terapia Fotodinâmica Antimicrobiana, FCT-PTDC/QUI-QUI/112595/2009, PI: Paulo Santos (CQVR), L.V. Reis (CQVR), 121 698 €

Estudo de modificações estruturais induzidas por degradação térmica e oxidativa de oligo e polissacarideos por espectrometria de massa, PTDC/QUI-QUI/100044/2008, 60 000 €

FCT Relatório Científico 2009 Print: 28-03-2010 23:13:39 [Centro de Química - Vila Real]

Group Description

Title of Research Group:	(RG-Norte-616-440) Materials Chemistry
Principal Investigator:	Verónica Cortés de Zea Bermudez
Main Scientific Domain:	Química
Group Host Institution:	Universidade de Trás-os-Montes e Alto Douro

Funding, source, dates

Funding, source, dates

Designing ultra-fine textured microstructures by laser floating zone - LaFlorZone, PTDC/CTM/66195/2006, P.B. Tavares, CQVR: 10 800 €. 2008/10.

Processing and Characterization of Multiferroic Ceramics for Sensors and Actuators, PTDC/CTM/67575/2006, P.B. Tavares, CQVR: 25 000 €. 2008/10.

Research on Magnetic and Multiferroic Oxides using Radioactive Isotopes at ISOLDE-CERN, CERN/FP/83643/2008. P.B. Tavares. CQVR: 4 000 €. 1/11/2008 - 31/10/2009.

Self-patternable organic/inorganic hybrids for low cost integrated optical devices.

POCTI/CTM/72093/2006: Industrial Partner: Siemens S.A., V.Z. Bermudez; CQVR: 10 984 € (2008/10)

F.C. Gulbenkian grant to visit D. Química Física, U.Barcelona. CQVR: 1200 €, R.M. Rego, 6/2009.

Multifunctional organic inorganic materials: nanostruturation via self-assembly and molecular recognition,. Acção Integrada Luso-Francesa, V.Z. Bermudez, M. W. Chi Man, CQVR: 7200 €

Synthesis of new tripodal silylated precursors, F. Oriente, RI Japan: K. Kuroda (Waseda U., Tokyo); RI (CQVR): V.Z. Bermudez; 2200 €; April-June 2009

Objectives & Achievements

Objectives

Organic/inorganic hybrid materials

To develop amorphous organic/inorganic hybrid systems derived from siliceous-based frameworks incorporating polyether-, or poly(e-caprolactone) (PCL)-type chains with variable length, containing urea or urethane cross-linkages and a wide range of guest salt/complex concentration. The species introduced include mono-, di- or trivalent cations aiming at imparting technologically important features to the final materials. Applications in the fields of advanced solid state batteries, electrochromic devices (ECDs), optics, and medicine were envisaged.

To develop organized hierarchically structured complex organic/inorganic hybrid materials by sol-gel procedures and self-assembly routes.

To develop via the sol-gel method biocompatible, biodegradable and photoluminescent biopolymer/siloxane hybrid scaffolds using different biopolymers and different cross-links. To achieve controlled growth of amorphous calcium carbonate (ACC) and ACC/biopolymer hybrid films on biopolymer/siloxane hybrid substrates for the creation of bio-inspired scaffolds with enhanced biocompatibility, improved biodegradability and tuneable mechanical, morphological and optical properties.

Ceramic and intermetallic materials

The multiferroic properties of ceramic systems like Bi1-xLaxFe1-yMnyO3, Eu1 xYxMnO3, Gd1-xYxMnO3, Eu1-xHoxMnO3 and Gd1-xHoxMnO3 will continue to be evaluated. In the case of BLMFO system we also intend to produce thin films by Pulsed Laser Deposition (first) and latter by RF-sputtering. To do this, high quality targets needed to be produced. A laboratory to measure film and bulk ceramic properties like polarization and leakage currents will start to be installed in collaboration with Physics Department of UTAD.

Collaborative investigation on the structural properties of the intermetallics Gd5Si2Ge2, PrNi5-xCox and Ni2Mn(Ga, Bi) systems will continue, due to the XRD and SEM facilities.

In 2009 the Laser Floating Zone system in Aveiro University will be fully operational. We will start by producing fibers and monocrystals of the Eu1-xYxMnO3 systems by that technique.

Catalysts

Different systems will be analysed: metal complexes, magnetic -Fe2O3@SiO2 nanoparticles, Metal/TiO2 and CeO2/Au nanoparticles. We will start the synthesis and characterization of alkoxysilane pentacoordinate oxovanadium(IV) complexes. These metal complexes will be anchored on SiO2 and Al2O3 as hybrid catalysts. Well characterized final catalysts will be applied for the hydro-isomerization and oxidation of hydrocarbons in micro batch reactor.

Metallic alloy materials

The development of fuel cells is dependent on the improvement of the gas diffusion electrodes (GDE). Their properties and designs are the key to control the reaction kinetics, mass transport and to avoid the poisoning of the catalyst surface during the fuel cell operation. It is thus our aim to develop a new architecture of cathode and anode gas diffusion electrodes:

Cathode – By using a non-powder type processes (electroless deposition) to produce nanoparticles of the catalyst, well anchored to the gas diffusion layer (carbon paper), and preferentially located nearby the surface layer. We expect that the new structure of the catalyst layer would decrease the sintering effect and the low catalyst efficiency usually found on powder type catalysts.

Anode – By producing a hydrogen-permeable electrode material, which would be in the form of a thin metallic thin film, placed between the gas feed and the electrolyte. This material would provide the route for hydrogen diffusion, electron conduction and site reaction, and would ensure simultaneously that the contaminants on the gas stream are physically separated from the electrolyte.

Objectives & Achievements

Main Achievements

Organic/inorganic hybrid materials

Prototype solid-state ECDs were successfully produced based on: (i) PEO/siloxane hybrid networks doped with Li-bis(trifluoromethanesulfonyl) imide (LiTFSI) and Li tetrafluoroborate (LiBF4) and (ii) PCL/siloxane hybrid networks doped with mixed triflate salts including Li+ and Eu3+ ions.

Highly luminescent di-ureasil hybrids doped with a Eu(III) complex including dipicolinate ligands and highly luminescent di-urethanesil hybrids doped with europium β-diketonate complexes containing either water ligands or a bulky chelating ligand were produced.

The inhibition of the formation of calcite through the use of several polymers with adequate functional groups was achieved by means of diamine compounds incorporating oxyethylene-based polymer segments of variable length. Aragonite and vaterite were formed in some cases.

Luminescent Lanthanide-containing 2,2'-Bipyridine-urea Bridged Urea Cross-linked Polysilsequioxanes were synthesized using self-assembly routes.

Ceramic Materials

Multiferroic properties were investigated in Eu1 xYxMnO3 and Gd1 xYxMnO3 ceramics. The results evidence a strong spin-phonon coupling in GdMnO3 and EuMnO3. The magnetoelectric effect is present in GdMnO3 but absent in EuMnO3 leading us to conclude that a spin-phonon coupling is not a sufficient condition for the existence of magneoelectric property. The composition Eu0.6Y0.4MnO3 presents a clear evidence for the influence of a magnetic field in the polar properties.

In the PrNi5-xCox it was observed that Co content has a strong influence on the Curie temperature changing from 60K (x=1.95) to 537 K (x=3). This series has an appreciable magnetocaloric cooling power, associated with the spin-reorientation process and Curie temperature Tc.

Catalysts

Newly synthesized alkoxysilane pentacoordinate oxovanadium(IV) complexes, VO[Sal(PMeOSi)DPTA] as 3[a], VO[Cl-Sal(PMeOSi)DPTA] as 3[b], VO[Sal(PMeOSi)DETA] as 6[a] and VO[Cl-Sal(PMeOSi)DETA] as 6[b] were anchored into SiO2 or Al2O3 as supported catalysts. The catalyst SiO2/3[a] system exhibits best activity for oxidation of cyclohexane (with O2), with an overall yield of 39% (TONs ca. 5.0 × 103) as well as high selectivity 98 %. Cyclohexane shows improved conversion 44 %, by the addition of carboxylic acid. The impact of radical traps and detection of intermediate peroxy radical were also investigated to establish a radical mechanism.

Well characterized pentacoordinate complexes of Cu[Sal(PMeOSi)DETA] and Co[Sal(PMeOSi)DETA], have been covalently bond with Al2O3 or SiO2 as hybrid catalysts. The SiO2/Cu catalyst shows best catalytic activity (for C6 conv. 25 % with selectivity 93 % at 150 ºC and for C7 conv. 20 % with selectivity 95 % at 160 ºC). We have obtained 2-ol, 3-ol as major products of C6 and C7 alkanes.

Metallic alloy materials

Cathode material: The methodology to deposit Pd on the carbon paper, by electroless deposition, was developed. The experimental conditions, in terms of the solution composition, time deposition and carbon paper pre-treatment (to suppress its hydrophobicity) were attained. The obtained deposits contained a Pd loading of 0.32 - 1.77 mg cm-2 and nanoparticles (16-20 nm) which were present as well dispersed clusters of 100-200 nm. It was found that prepared catalysts exhibit a high catalytic activity towards the oxygen reduction reaction, comparable to Pt. This material was tested on a PEM fuel cell, as the cathode material, but due to its high hydrophilicity it was flooded by the water coming from the gas stream.

Anode material: The methodology to deposit Pd-Ag alloys on a disc of stainless steel, by electroless deposition, was developed. The experimental conditions, solution composition, time, annealing and temperature, were attained. It was found that unless an oxide film was previously formed on the stainless steel substrate, Pd alloys containing Fe, Ni and/or Cr, instead of Ag, would be formed. Films of Pd-Ag alloys containing 34 to 7 % at. of Ag were prepared.

Group Productivity

Publications in peer review Journals

L. D. CARLOS, R. A. S. FERREIRA, V. DE ZEA BERMUDEZ, S. J. L. RIBEIRO, (2009) "Lanthanide-containing light-emitting organic-inorganic hybrids: a bet on the future", Advanced Materials, 5, 1-26. Invited Review Article (IF= 8.191)

P. P. LIMA, F. A. ALMEIDA PAZ,. R. A. S. FERREIRA, V. DE ZEA BERMUDEZ, L. D. CARLOS, (2009) "Highly luminescent Eu3+–containing organic–inorganic hybrids formed through ligands–assisted rational design", Chemistry of Materials, 21(21), 5099–5111. (IF= 5.046)

S. M. F. VILELA, F. A. ALMEIDA PAZ, J. P. C. TOMÉ, V. DE ZEA BERMUDEZ, J. A. S. CAVALEIRO, J. ROCHA, (2009) "Methyl 2-(4,6-dichloro-1,3,5-triazin-2-ylamino)acetate", Acta Crystallographica, E65, 1985-1986. (IF= 0.367)

S. M. F. VILELA, F. A. ALMEIDA PAZ, J. P. C. TOMÉ, V. DE ZEA BERMUDEZ, J. A. S. CAVALEIRO, J. ROCHA, (2009) "Glycine methyl ester hydrochloride", Acta Crystallographica, E65, 1985-1986. (IF= 0.367)

P. C. BARBOSA, M. M. SILVA, M. J. SMITH, A. GONÇALVES, E. FORTUNATO, S. C. NUNES, V. DE ZEA BERMUDEZ, (2009) "Di-ureasil xerogels containing lithium bis(trifluoromethanesulfonyl)imide for application in solid-state electrochromic devices", Electrochimica Acta 54,1002-1009. (IF= 3.078)

M. FERNANDES, S. S. NOBRE, M. C. GONÇALVES, A. CHARAS, J. MORGADO, R. A. S. FERREIRA, L. D. CARLOS, V. DE ZEA BERMUDEZ, (2009) "Dual role of a di-urethanesil hybrid doped with europium β-diketonate complexes containing either water ligands or a bulky chelating ligand", Journal of Materials Chemistry, 19, 733-742. (IF= 4.646)

M. E. MESQUITA, S. S. NOBRE, M. FERNANDES, R. A. S. FERREIRA, SÍLVIA C. G. SANTOS, MARCELO O. RODRIGUES, L. D. CARLOS, V. DE ZEA BERMUDEZ, (2009) "Highly luminescent di-ureasil hybrid doped with a Eu(III) complex including dipicolinate ligands, Journal of Photochemistry and Photobiology A, Chemistry, 205 (2-3), 156-160. (IF= 2.362)

W. S. FERREIRA, J. AGOSTINHO MOREIRA, A. ALMEIDA, M. R. CHAVES, J. P. ARAÚJO, J. B. OLIVEIRA, J. M. MACHADO DA SILVA, M. A. SÁ, T. M. MENDONÇA, P. SIMEÃO CARVALHO, J. KREISEL, J. L. RIBEIRO, L. G. VIEIRA, P. B. TAVARES, S. MENDONÇA, (2009) "Spin-phonon coupling and magnetoelectric properties: EuMnO3 versus GdMnO3" Physical Review B 79, p. 54303-1-10. (IF= 3.322)

D.L. ROCCO, J.S. AMARAL, J.V. LEITÃO, V.S. AMARAL, M.S. REIS, R.P. FERNANDES, A.M. PEREIRA, J.P. ARAÚJO, NUNO V. MARTINS, P.B. TAVARES, A.A. COELHO, (2009) "Percolation processes and spin reorientation on PrNi5-xCox", Physical Review B 79, p. 014428-1-6. (IF= 3.322)

D L ROCCO, J S AMARAL, J V LEITÃO, V S AMARAL, M S REIS, SOMA DAS, R P FERNANDES, J P ARAÚJO, A M PEREIRA, P B TAVARES, NUNO V

Group Productivity

MARTINS AND A A COELHO (2009) "High refrigerant capacity of PrNi5-xCox magnetic compounds exploiting its spin reorientation and magnetic transition over a wide temperature zone", J. Phys. D: Appl. Phys. 42, p.055002-1-4. (IF= 2.104)

J. AGOSTINHO MOREIRA, A. ALMEIDA, W.S. FERREIRA, M.R. CHAVES, B. KUNDYS, R. RANJITH, W. PRELLIER, S.M.F. VILELA, P.B. TAVARES (2009) "Polar properties of Eu0.6Y0.4MnO3 ceramics and their magnetic field dependence" J.Phys.: Condens. Matter. 21, 446002 (10 pp). (IF= 1.900)

REGO, ROSA; OLIVEIRA MARIA; ESPARBÉ, ISAAC; CABOT, PERE (2009) – "Development of Pd-based membranes as hydrogen diffusion anodes", J. Power Sources, 189: 1120-1126. (IF=3.477)

Other publications International

BOOKS:

CARLOS L. D., SÁ FERREIRA R. A., DE ZEA BERMUDEZ V. Organic/Inorganic hybrids for light-emitting devices and integrated optics. Em Hybrid Nanocomposites for Nanotechnology: Electronic, Optical, Magnetic and BioMedical Applications. Lhadi Merhari (Ed.), Springer, New York, 2009, Part III, pgs. 509-586. ISBN-10: 0387723986

Proceedings or extended abstracts:

FERNANDES M., NOBRE S. S., RODRIGUES L. C., BARBOSA P. C., FERREIRA R. A. S., SILVA M. M., CARLOS, L. D., DE ZEA BERMUDEZ V. "PCL(530)/siloxane biohybrids doped with Li+ and Eu3+". HYCELTEC 2009 - II Iberian Symposium on Hydrogen, Fuel Cells and Advanced Batteries, Vila Real, 13-17 September 2009. Book of Extended Abstracts, P04-SC

GOPAL S. MISHRA, ANIL KUMAR, PEDRO B. TAVARES, "Cobalt, Cupper and Vanadium Complexes Covalently Linked with Silica as Supported Catalysts for Oxidation of Cyclohexane by Dioxygen", 6th World Congress on Oxidation Catalysis, July 5-10, 2009 Lille-France, 2A-862, p. 212-213.

BRUNO SILVA, FERNANDO NUNES, AMANDIO PINTO, PEDRO TAVARES, HUMBERTO VARUM, JORGE PINTO. Perspectiva biomimética do ninho de andorinha-dos-beirais. CD do VIII Seminario Iberoamericano de Construcción com Tierra (VIII SIACOT) e do II Seminario Argentino de Arquitectura y Construcción com Tierra (II SAACT). Editor: CRIATIAC – FAU – UNT. Junho de 2009. Tucumán, Argentina. pag. 326-332. Junho de 2009.

BRUNO SILVA, FERNANDO NUNES, AMANDIO PINTO, PEDRO TAVARES, HUMBERTO VARUM, JORGE PINTO. Perspectiva biomimética do ninho de andorinha-dos-beirais. Livro de Publicações de Resumos do VIII Seminario Iberoamericano de Construcción com Tierra (VIII SIACOT) e do II Seminario Argentino de Arquitectura y Construcción com Tierra (II SAACT). Editor: CRIATIAC – FAU – UNT. Junho de 2009. Tucumán, Argentina. pag. 100-101. Junho de 2009.

PINTO, J.; VARUM, H.; CRUZ, D.; SOUSA, D.; MORAIS, P.; TAVARES, P.; LOUSADA, J.; SILVA, P.; VIEIRA, J. ;2009 ; Tabique Construction Characterization in Douro North Valley, Portugal: A First Step to Preserve this Architectural Heritage - 2nd WSEAS International Conference on Urban Rehabilitation and Sustainability (URES'09) - Environmental Science and Sustainability - Proceedings published by WSEAS Press (printed and in CD), Editors: Manoj Jha, Charles Long, Nikos Mastorakis, Cornelia Aida Bulucea, ISBN 978-960-474-136-6, ISSN 1790-5095, pp. 48-53 - Baltimore, USA, 7-9 Novem-ber of 2009.

SILVA, B.; CORREIA, J.; NUNES, F.; TAVARES, P.; VARUM, H.; PINTO, J. ;2009 ; - Earth Construction: Bird Teaching - 2nd WSEAS International Conference on Urban Rehabilitation and Sustainability (URES'09), Environmental Science and Sustainability - Proceedings published by WSEAS Press (printed and in CD), Editors: Manoj Jha, Charles Long, Nikos Mastorakis, Cornelia Aida Bulucea, ISBN 978-960-474-136-6, ISSN 1790-5095, pp. 72-78 - Baltimore, USA, 7-9 November of 2009.

Other publications National

CONSTANTE D., PINHO J., FERNANDES M., DE ZEA BERMUDEZ V., Precipitação biomimética de carbonato de cálcio amorfo em meio polimérico: estudo do efeito do polímero", 3as Jornadas de Biologia, UTAD, Vila Real, 21-22 October 2009, Book of Abstracts, p. 37.

CONSTANTE D., FERNANDES M., DE ZEA BERMUDEZ V. "Bio-inspired growth of amorphous calcium carbonate on polyether-based diamines", 1as Jornadas de Bioengenharia da FEUP, Porto, 27 and 28 November 2009, Book of Abstracts, p. 45

JULIANA OLIVEIRA, J. AGOSTINHO MOREIRA, LUÍS FERREIRA, A. ALMEIDA, P.B. TAVARES AND S. VILELA (2009) "Dipolar relaxation process in Eu1-xLuxMnO3 ceramics", IJUP 09 – 2nd Meeting of Young Researchers at UP, Universidade do Porto, 25-27 Feb., Book of abstracts p. 173.

J. OLIVEIRA, J. AGOSTINHO MOREIRA, W. S. FERREIRA, A. ALMEIDA, P. B. TAVARES, S. VILELA (2009) "Dipolar relaxation process in Eu1-xLuxMnO3 ceramics, 2nd Workshop of the Associated Laboratory "Institute of Nanoscience and Nanotechnology" (IN) 20 October 2009, Instituto Superior Técnico (Book of abstracts).

J. AGOSTINHO MOREIRA, A. ALMEIDA, W. S. FERREIRA, M. R. CHAVES, J. KREISEL, S. M. F. VILELA, P. B. TAVARES (2009), "Coupling between phonons and magnetic excitations in orthorhombic Eu1-xYxMnO3", 2nd Workshop of the Associated Laboratory "Institute of Nanoscience and Nanotechnology" (IN) 20 October 2009, Instituto Superior Técnico (Book of abstracts).

W. S. FERREIRA, J. AGOSTINHO MOREIRA, A. ALMEIDA, M. R. CHAVES, J. P. ARAÚJO, J. B. OLIVEIRA, J. M. MACHADO DA SILVA, M. A. SÁ, T. M. MENDONÇA, P. SIMEÃO CARVALHO, P. B.TAVARES (2009) "Spin-phonon coupling and magnetoelectric properties: EuMnO3 versus GdMnO3", 2nd Workshop of the Associated Laboratory "Institute of Nanoscience and Nanotechnology" (IN) 20 October 2009, Instituto Superior Técnico (Book of abstracts).

Master and Ph.D. thesis completed

Master completed

Contributo para a Avaliação do Comportamento Geotécnico das Argilas Sobreconsolidadas de Leiria – DAVID AUGUSTO COELHO ARMINDO, Master Thesis, UTAD, 9/3/2009, under the supervision of Amândio Teixeira Pinto (CQVR) and Anabela Veiga (IPL).

Estabilização Superficial de Solos Argilosos por Activação Alcalina – sua Aplicação em Bases de Pavimentos, BRUNO SEQUEIRA NOGUEIRA, Master Thesis, UTAD, 9/3/2009, under the supervision of Amândio Teixeira Pinto (CQVR).

Group Productivity

PhD completed

Deep Soft Soil Improvement by Alkaline Activation, NUNO MIGUEL CORDEIRO CRISTELO, in University of Newcastle-upon-Thyne England, April/2009 , under the supervision of Sthephanie Glenndinning and Amândio Teixeira Pinto (CQVR).

Patents/propotypes

Submeted:

GOPAL S. MISHRA, P. B. TAVARES, ANIL KUMAR

Catalisadores Híbridos de Vanádio e sua Utilização em Processos de Oxidação Selectiva de Cicloalcanos. Pedido de Invenção Nacional N.º 104862, 28/09/2009, Requested PCT Nº. PCT/IB2009/055665.

A. TEIXEIRA PINTO, P.B. TAVARES, "Processo para a Obtenção de Produtos de Reciclagem de Resíduos de Vidro e de Lamas de Estações de Tratamento de Água, Ricas em Alumínio, e Produtos Assim Obtidos", Patente de Invenção Nacional N.º 104535, 27/04/2009.

A. TEIXEIRA PINTO, BRUNO NOGUEIRA, "Estabilização de Solos por Activação Alcalina", Patente de Invenção Nacional N.º 104421, 26/04/2009.

Organization of conferences

Hyceltec 2009, II Iberian Symposium on Hydrogen Fuel Cells and Advanced Batteries, Vila Real, 13-17 September 2009 (http://www.hyceltec2009.utad.pt/en/welcome.html).

CQVR members in the organization committee: V.B. Bermudez, M.C. Oliveira, R. Rego, M.C. Gonçalves. BII's, MSc and PhD Students of the Materials Chemistry group: José Teixeira (Undergraduate Student), Mariana Fernandes (PhD Student), Sérgio Vilela (MSc Student), Sílvia Nunes (Post-Doc Student), Teresa Carvalho (PhD Student), João Pinho (Undergraduate Student), Diogo Constante (Undergraduate Student), Lisete Fernandes (UME Technician).

Internationalization

Traineeships periods and collaborative publications with Laboratoire CRISMAT, UMR 6508 CNRS/ENSICAEN, France (W. Prellier).

Collaborative publications with LMGP, CNRS, Grenoble Institute of Technology, France (J. Kreisel).

Collaborative publications with Instituto de Física Gleb Wataghin, UNICAMP, Campinas, S. Paulo, Brasil

Collaborative publications with Dep. Física, Universidade Federal de Ouro Preto, MG, Brasil.

Collaborative publications with École de Chimie de Montpellier (Montpellier, France) (M. W.Chi Man)

Collaborative publications with Departamento de Química de Araraquara, UNESP (Araraquara, São Paulo, Brasil (S. Ribeiro)

Collaborative publications with Prof. Anil Kumar, Chemical Engineering Department, Indian Institute of Technology Kanpur, Kanpur-208016, India

Traineeships period and collaborative work with Department of Applied Chemistry, Waseda University (Professor Kazayuki Kuroda) and Professor Atsushi Shimojima (Department of Chemical System Engineering, The University of Tokyo), Tokyo, Japan

Traineeships periods and collaborative publications with Depart. de Química Física, Facultat de Química, Universitat de Barcelona. (P. L. Cabot).

Collaboration in the Joint European Masters in Material Science EMMS, Univ. Aveiro, Technische Universitat Hamburg-Harburg, Aalborg Univ., P.B. Tavares, V.de Zea Bermudez.

Sócrates/Erasmus Program (Acção I) 210377-IC-1-2000-1-FR-ERASMUS-IP-1 (2008-2013)

Institutions and PI:

Institute für Anorganische Chemie, U. Wien, Austria – A. Mikula

Institut für Chemische Physik fester Stoffe, TH Dresden, Alemanha – M. Ruck

Institut de Ciencia Molecular, U. de Valencia, Espanha – C. G. Garcia

FMC, U. de Cantábria, Santander, Espanha - J. Gomez Sal

ICMA, U. de Zaragoza, Espanha - Juan Bartolomé

U. Joseph Fourier, Grenoble, França - Michel Duclot - Coordenador

U. Joseph Fourier, Grenoble, França - Jean-Claude Marmeggi

Aristotle U., Salonika, Grécia - George Litsardakis

U. degli Studi di Roma "La Sapienza", Itália - Franco Decker

U. degli Studi di Genova, Itália - Gabriella Borzone

U. degli Studi di Pavia, Itália - Paolo Ferloni

U. Twente, Holanda – M. Podt

FCUL, Portugal – C. Cruz

ITN, Portugal – M. Almeida

FCUL, Portugal – M. Godinho

Academia Militar, Portugal – T. Gasche

UTAD, Portugal – V. de Zea Bermudez

University of Ljubliana, Eslovénia – B. Orel

Linköpings U., Suécia – S. Johansson

Group Productivity

De Montford U., Leicester, UK – W. Schlindwein

Future Research

Objectives

Organic/inorganic hybrid materials

To pursue the development of amorphous organic/inorganic hybrid systems derived from siliceous-based frameworks incorporating biopolymers with variable length, containing urea or urethane cross-linkages and a wide range of guest salt/complex concentration. The species introduced include mono-, di- or trivalent cations aiming at imparting technologically important features to the final materials.

Several ionic liquids will be grafted to the inorganic skeleton or simply added with the goal of enhancing the ionic conductivity.

Applications in the fields of advanced solid state batteries, electrochromic devices, optics, and medicine are envisaged.

To pursue the investigation of organized hierarchically structured complex organic/inorganic hybrid materials by sol-gel procedures and self-assembly routes and in particular get better insight into the influence of cation doping and solvent medium on the morphology, structure and properties of the resulting materials (in particular the order/disorder phase transition temperature) using alkyl-based mono-amide and mono-urethane cross-linked alkylsilanes and di-urea cross-linked silsesquioxanes as starting precursors.

To pursue the biomineralization/biomimetic studies using different high molecular weight polymers to control the growth of amorphous calcium carbonate (ACC) and ACC/biopolymer hybrid films on biopolymer/siloxane hybrid substrates and thus inhibit the formation of calcite in the early stages of crystallisation for the creation of bio-inspired scaffolds with enhanced biocompatibility, improved biodegradability and tuneable mechanical, morphological and optical properties. Applications in the field of Orthopedics are foreseen.

Ceramic materials

To pursue the synthesis and characterization of ceramic materials for sensors and actuators, in particular those with potential multiferroic properties, Eu0.8Y0.2MnO3 composition will be deeply studied due to its very distinctive phase diagram, where it is still poorly understood the actual ferroelectric character of the low temperature magnetic phases. We will study in detail the temperature dependence of the electric polarization of Eu0.8Y0.2MnO3 aimed at clarifying the controversial issues concerning the ferroelectric nature of the lower temperature magnetic phases and hence its multiferroic character. In order to figure out what is the origin of the microscopic mechanisms that drive its behaviour, we will carried out a detailed study of the displacement currents for both different starting conditions and polarizing electric fields, and of the field dependent of the magnetodielectric effect. Deep structural characterizations will be performed applying Rietveld analysis on XRD data obtained at different temperatures (5-300 K).

A large effort will be done on the preparation and characterization of targets and thin films by RF-Sputtering in the Bi1-xLaxFe1-yMnyO system.

A new laboratory for measuring electric properties (polarization and leakage currents as a first objective) will be installed in collaboration with the Physics Dep. of UTAD.

Catalysts

New metal complexes, hybrid and magnetic nano-materials catalysts will continue to be synthesised, characterized and their catalytic behaviour will be tested.

In the metal complexes we intend to follow the synthesis and crystallization of new tris-pyrazoyl ethanol Pd, Au, V complexes and pentacoordinate Mn, Fe complexes covalent bonded by grafting method on the surface of modified mesoporous materials (MCM-41, SBA-15, Nano-size materials). These Hybrid catalysts will be tested for oxidation of alkanes with dioxygen and reformation of linear hydrocarbons (light naphtha) to branch isomers to increase the burning efficacy of fuel. Both the oxidation and isomerization reactions are optimize for best reaction condition.

VO(acac)2 will be immobilazed in superparamagnetic -Fe2O3 coated by silica shells and functionalized by amine groups, and tested in the epoxidation of geraniol. The catalyst will be easily recovered by magnetic separation.

Ultrafine cubic CeO2 particles will be prepared by a solvothermal method, and compared with a commercial CeO2. Au will be loaded onto the obtained ceria supports by a double impregnation (DIM) method. Activities for CO oxidation will be compared. The effect of the presence of chloride on the sinterization of Au/CeO2 catalysts will be investigated.

Metallic alloy materials

To pursue the investigation on new electrode materials for the cathode and anode of fuel cells.

Cathode: The methodology to deposit Pd and Pd-P alloys nanoparticles on carbon paper impregnated with hydrophobic material (Teflon) will be developed, in order to envisage the application of these materials to low temperature fuel cells.

The influence of some experimental deposition parameters, such as the electroless bath composition, on the Pd grain size will be analysed by SEM and TEM.

The activity of the prepared electrodes towards the O2 reduction, and towards methanol and ethanol oxidation, in acid and alkaline medium will be evaluated by electrochemical techniques. The prepared material will be testes on a PEMFC, DMFC and DEFC.

Anode material: The activity of the prepared electrodes (Pd-Ag alloys) towards the H2 oxidation, methanol and ethanol oxidation, in acid and alkaline medium, will be evaluated and the tolerance of the prepared material to CO will be compared.

The Pd-Ag films exhibiting the highest electroactivity and CO tolerance will be deposit on a porous stainless steel envisaging its application to low temperature fuel cells.

Funding, source, dates

Self-patternable organic/inorganic hybrids for low cost integrated optical devices.

POCTI/CTM/72093/2006, CQVR: 10 984 € (2008-2010)

Híbridos orgânicos-inorgânicos com propriedades de emissão optimizadas para aplicação na nova geração de comunicações ópticas. PTDC/CTM /101324/2008, CQVR funding: 36 182 € (2010-2012).

Designing ultra-fine textured microstructures by LFZ, PTDC/CTM/66195/2006, 10 800 €. (2008-2010).

Processing and Characterization of Multiferroic Ceramics for Sensors and Actuators, PTDC/CTM/67575/2006, CQVR: 25 000 €. (2008-2010).

Future Research

MULTIFOX: Nanometric Probing and Modification of Multiferroic Oxides, PTDC/FIS/105416/2008, CQVR: 14 400 € (2010-2013)

Multiferroics and magnetoelectrics for spintronics: barriers and interfaces, PTDC/CTM/099415/2008, CQVR: 29 232€ (2010-2012)

Estudos de Materiais Magnéticos e Multiferróicos utilizando Isótopos Radioactivos no ISOLDE-CERN, CERN/FP/109357/2009, CQVR: 3 600€ (2010-2011).

Pending funds

Bio-inspired deposition of a biomineral for biomedical applications, PTDC/CTM/102098/2008. 131 268 €

Innovative Materials for Electrochromic Applications, PTDC/QUI/105281/2008 46 440 €

Organic-inorganic hybrids for biomedical sensing, PTDC/CTM/111361/2009, 25 176 €

Study of the spin-phonon coupling in magnetoelectric manganites, PTDC/FIS/110936/2009, 39 888 €

Development of CO tolerant anodes for fuel cells, PTDC/CTM/109958/2009, 126 255 €

A novel route to prepare Pd and Pd-based nanocatalyst", PTDC/QUI/110855/2009, 187.938 €

Mesoporous material supported in metal complexes catalysts, PTDC/EQU/110825/2009.

FCT Relatório Científico 2009 Print: 28-03-2010 23:15:06 [Centro de Química - Vila Real]

Group Description

Title of Research Group:	(RG-Norte-616-1509) Environmental Chemistry
Principal Investigator:	Jose Alcides Silvestre Peres
Main Scientific Domain:	Química
Group Host Institution:	Universidade de Trás-os-Montes e Alto Douro

Funding, source, dates

Funding, source, dates

SUVIDUR – Sustentabilidade da viticultura de encosta nas regiões do Douro e do Duero. INTERREG/POCTEP, 411 433 € (2009/2011)

BioCombus – Recovery of Wastes as Bio Fuel - a process for the treatment and recovery of wastes and effluents from olive oil production units, FP7 Nº 3483, 1 168 574 €. (10/2008 - 09/2011).

Winery wastewater treatment by a combination of chemical and biological processes. Supported by ATMAD, 24 000 €. (05/2006 - 04/2010).

Development of new fertilizers to agriculture, in collaboration with CUF, Adubos de Portugal. 10 000 €/year. (2009)

Modelling nitrogen mineralization in Eucalyptus globulus stands, in collaboration with RAIZ, Instituto de Investigação da Floresta e do Papel, 10 000 €/year (2009)

Effect of phytochemicals on the organic residues transformation and on key processes of the C and N cycles. PTDC/AGR-AAM/102006/2008, €125 680,00

Objectives & Achievements

Objectives

Environmental pollution constitutes one of the main concerns of modern societies. Great care has been devoted to this subject and all the solutions are based on a working philosophy of reduce, reuse and recycle. The main objectives are:

1. Study different Advanced Oxidation Processes (AOPs) to reduce the phenolic compounds present in problematic wastewaters, like winery wastewaters, olive mill wastewaters, textile wastewaters and enhanced treatment processes. Our objective is study combined chemical-biological or AOP-coagulation/flocculation treatment approaches to be applied in effluents that are refractory to conventional treatments.

2. Compare the effectiveness of adsorbent prepared from for removal endocrine disruptors compounds and pesticides from water.

3. Study the occurrence of ocratoxin A and ethyl carbamate (urethane) in winery by-products.

4. To study the influence of time scale on geochemical processes.

• understanding of processes leading groundwaters to their chemical composition and quantify mineral weathering rates, especially of plagioclases, at watershed scale. Understanding the role of time (duration of a weathering episode) in the estimated rates.

5. Research on treatment, recovery and valorisation of industrial by-products and wastes under an industrial ecology approach.

6. To study nitrogen and carbon turnover after organic amendment application to soils in order to predict nitrogen availability to crops and/or nitrate leaching risks.

To propose a laboratory method to study phosphorus desorption isotherms in agricultural soils. To study the effect of slurry acidification on phosphorus dynamics, after soil application.

Main Achievements

1. Phenolic acids ozonation were studied by QSAR analysis and the influence of pH on the selectivity of ozone. Kinetic studies of olive mill wastewater treatment by a simple process (Fenton's reagent) and by a combined process (Fenton's reagent and chemical coagulation) were developed. In a practical point of view, winery wastewaters were successfully treated: (1) using a pilot-scale bubble column ozonation reactor; (2) using a solar Compound Parabolic Collector (CPC) photo-Fenton reactor and (3) combining long term aerated storage (biological process) and Fenton's reagent. Finally, we developed a photochemical degradation study of three commercial azo dyes used in the textile industry.

2. Adsorbents prepared from pine bark and almond shell are effective for the removal of Bisphenol A and 17β- estradiol from aqueous solutions. The effect of particle size was found to be of considerable significance, for all adsorbents the percentage removal of both disruptors decreased with the increasing particle size. The experimental results also displayed that the treatment affect the adsorption capacity. Pine bark and almond shell powders pretreated with formaldehyde presented higher adsorption efficiency, followed by pine bark and almond shell washed with hot water.

3. The presence of ethyl carbamate (EC) in marc brandies was investigated by GC-MS, using two extraction procedures. After the removal of ethanol, solid-phase microextraction (SPME) and solid-phase extraction (SPE) were optimized using spiked marc brandy samples. The limits of detection attained by SPME/GC-MS and SPE/GC-MS were 10 and 30 μgL-1, respectively. SPME procedure yields a recovery range from 91 to 108%, while the SPE provide values from 89 to 112%. The quantification of EC in the samples with amounts above the detection limit indicates levels between 10 and 160 μgL-1. A good agreement of analytical results was observed for both procedures. For the commercial marc brandy samples analysed, no correlation between aging time or geographical origin was observed regarding to the EC amount.

4. New patent registration. Licence Agreement for technology transfer of patent process. Implementation of the patented technologies, namely in the ambit of the BioCombus project.

5. Development and application of models suitable to study mineral weathering rates under field conditions, taking into account the main factors. Models were successfully applied and results demonstrate that contemporary weathering rates estimated at the watershed scale in several places in Portugal follow the trend of rates obtained in the laboratory during experiments run over fresh material, being much larger than rates obtained at the soil profile scale where saprolite materials are studied. Eventually, this is a result of differences in the duration of a soil formation episode relative to a watershed development episode.

Objectives & Achievements

6. Development of the main guidelines for the methodology to assess carbon and nitrogen processes and mineralization in soils and to predict carbon sequestration, nitrogen availability and nitrate leaching risks are studied. Effect of antropic contaminants on the microbial activity of the soils and C and N cycles.

Laboratory methods based on the use of anion exchange resins were tested such as guidelines for a new methodology to study phosphorus desorption isotherms in agricultural soils. Desorption isotherms area a major tool to characterize the factors that control soil solution P concentration and thus to predict plant P availability and environmental risks such as P leaching.

A fractionation method was used to follow inorganic and organic soil phosphorus transformations when slurries submitted to different management practices were applied to soil.

Group Productivity

Publications in peer review Journals

DOMÍNGUEZ, J.R.; PERES, J.A.; BELTRAN-HEREDIA, J.; "Phenolic acids ozonation: QSAR analysis and pH influence on the selectivity of ozone", Journal of Advanced Oxidation Technologies, 12 (2), 249-254 (2009). (IF= 0.495)

FANGUEIRO, D.; FERNANDES, A.; COUTINHO, J.; MOREIRA, N.; TRINDADE, H. (2009) - Influence of two nitrification inhibitors (DCD and DMPP) on annual ryegrass yield and soil mineral n dynamics after incorporation with cattle slurry. Communications in Soil Science and Plant Analysis, 40: 3387–3398. (IF= 0.357)

FANGUEIRO, D.; RIBEIRO, H.; VASCONCELOS, E.; COUTINHO, J.; CABRAL, F. (2009) - Treatment by acidification followed by solid–liquid separation affects slurry and slurry fractions composition and their potential of N mineralization. Bioresource Technology, 100: 4914–4917. (IF= 4.453)

LUCAS, M.S.; Mosteo, R.; Maldonado, M.I.; Malato, S.; PERES, J.A. Solar photochemical treatment of winery wastewater in a CPC reactor. Journal of Agricultural and Food Chemistry. 57, 11242-11248 (2009). (IF=2.562)

LUCAS, M.S.; Mouta, M.; PIRRA, A.; PERES J.A. Winery wastewater treatment by a combined process: long term aerated storage and Fenton's reagent. Water Science and Technology. 60, 1089-1095 (2009). (IF= 1.005)

LUCAS, M.S.; PERES, J.A. Removal of COD from olive mill wastewater by Fenton's reagent: kinetic study. Journal of Hazardous Materials, 168, 1253–1259 (2009). (IF= 2.975)

LUCAS, M.S.; PERES, J.A. Treatment of olive mill wastewater by a combined process: Fenton's reagent and chemical coagulation, Journal of Environmental Science and Health, Part A, 44, 198-205 (2009). (IF= 1.002)

LUCAS, M.S.; PERES, J.A.; Lan B.Y.; Li Puma G. Ozonation kinetics of winery wastewater in a pilot-scale bubble column reactor. Water Research. 43, 1523-1532 (2009). (IF= 3.587)

MOUTINHO-PEREIRA, J.; GONÇALVES, B.; BACELAR, E.; BOAVENTURA CUNHA J.; COUTINHO, J.; CORREIA, C. (2009) - Effects of elevated CO2 on grapevine (Vitis vinifera L.): physiological and yield attributes. Vitis, 48: 159-165. (IF= 0.795)

SOUSA, J.R.; COUTINHO, J. (2009) - Effect of the extraction period on the routine assessment of soil p status by ion-exchange resin membranes. Communications in Soil Science and Plant Analysis, 40: 1995 – 2008. (IF= 0.357)

TRINDADE, H.; COUTINHO, J.; JARVIS, S.; MOREIRA, N. (2009) - Effects of different rates and timing of application of nitrogen as slurry and mineral fertilizer on yield of herbage and nitrate-leaching potential of a maize/Italian ryegrass cropping system in north-west Portugal. Grass and Forage Science, 64: 2-11. (IF= 1.378)

Other publications International

Proceedings

BRITO, Luís Miguel; AMARO, A.L.; MOURÃO, Isabel Maria; COUTINHO, João, (2009) - Nitrogen transformation and organic matter mineralisation during composting screw pressed cattle slurry with oat straw. In: C. Grignani, M. Acutis, L. Zavattaro, L. Bechini, C. Bertora, P. Marino Gallina, D. Sacco (Eds). Proceedings of the 16th Nitrogen Workshop: Connecting different scales of nitrogen use in agriculture, Univ Milan, Turim, 351-352.

CABRAL, Fernanda; FANGUEIRO, David; VASCONCELOS, Ernesto; RIBEIRO, Henrique; COUTINHO, João (2009) - Pig slurry treatment by acidification followed by solid-liquid separation: Characteristics and Potential N mineralization of slurry fractions obtained. In: C. Grignani, M. Acutis, L. Zavattaro, L. Bechini, C. Bertora, P. Marino Gallina, D. Sacco (Eds). Proceedings of the 16th Nitrogen Workshop: Connecting different scales of nitrogen use in agriculture, Univ Milan, Turim, 245-246.

CARNEIRO, João; COUTINHO, João; TRINDADE, Henrique (2009) - Evaluation of N2O emissions from different organic residues incorporated to soil under Mediterranean conditions. In: C. Grignani, M. Acutis, L. Zavattaro, L. Bechini, C. Bertora, P. Marino Gallina, D. Sacco (Eds). Proceedings of the 16th Nitrogen Workshop: Connecting different scales of nitrogen use in agriculture, Univ Milan, Turim, 131-132.

FANGUEIRO, David; CABRAL, Fernanda; VASCONCELOS, Ernesto; RIBEIRO, Henrique; COUTINHO, João (2009) – Effect of pig slurry treatment by acidification followed by solid-liquid separation on nitrogen mineralization after application to soil. In: C. Grignani, M. Acutis, L. Zavattaro, L. Bechini, C. Bertora, P. Marino Gallina, D. Sacco (Eds). Proceedings of the 16th Nitrogen Workshop: Connecting different scales of nitrogen use in agriculture, Univ Milan, Turim, 357-358.

Gomes, M. E.P., Antunes, I.M.H.R., PACHECO, F.A.L., Silva, P.B., Neiva, A.M.R. (2009). Geochemistry of minerals, weathering and hidrogeochemistry from the Fonte Santa mine area (NE de Portugal). VII Congresso Ibérico e X Congresso Nacional de Geoquímica, Colégio Oficial e Associação de Químicos de Madrid, Soria, Espanha, 21 a 23 de Setembro de 2009, p. 251-260 (in CD).

LUCAS M.S., Mosteo R., Maldonado M.I., Malato S., PERES J.A. Photochemical treatment of a winery wastewater in a solar pilot plant. 5th International specialized conference on sustainable viticulture: winery waste and ecologic impacts in management. Trento and Verona. Italy, 30th March – 3rd April 2009. Proceedings book ISBN 978-88-8443-284-1, pp. 109-115.

LUCAS M.S., Mouta M., Pirra A., PERES J.A. Winery wastewater treatment by a combined process: long term aerated storage and Fenton's reagent.

Group Productivity

5th International specialized conference on sustainable viticulture: winery waste and ecologic impacts in management. Trento and Verona. Italy, 30th March – 3rd April 2009. Proceedings book ISBN 978-88-8443-284-1, pp. 99-107.

LUCAS M.S., PERES J.A., Li Puma G. Treatment of winery wastewater with ozone, ozone/UV and ozone/UV/H2O2. 5th International specialized conference on sustainable viticulture: winery waste and ecologic impacts in management. Trento and Verona. Italy, 30th March – 3rd April 2009. Proceedings book ISBN 978-88-8443-284-1, pp. 429-432.

MENDES, Susana; FANGUEIRO, David; CABRAL, Fernanda; COUTINHO, João, (2009) - Assessment of the potential N mineralization from different pig slurry particle size fractions using a short-time incubation method. In: C. Grignani, M. Acutis, L. Zavattaro, L. Bechini, C. Bertora, P. Marino Gallina, D. Sacco (Eds). Proceedings of the 16th Nitrogen Workshop: Connecting different scales of nitrogen use in agriculture, Univ Milan, Turim, 261-262.

PACHECO, F.A.L.; Medina, J., Ribeiro, S.; Van der Weijden, C.H. (2009). Duration of Weathering Episodes in Small Watersheds: Implication on Plagioclase Weathering Rates. VII Congresso Ibérico e X Congresso Nacional de Geoquímica, Colégio Oficial e Associação de Químicos de Madrid, Soria, Espanha, 21 a 23 de Setembro de 2009, p. 282-292 (in CD).

PEREIRA, José; FANGUEIRO, David; CHADWICK; David; MISSELBROOK, T.H.; COUTINHO, João; TRINDADE, Henrique (2009) – Influence of cattle slurry treatment by separation and nitrification inhibitors addition on N dynamics and N2O emissions after soil application. In: C. Grignani, M. Acutis, L. Zavattaro, L. Bechini, C. Bertora, P. Marino Gallina, D. Sacco (Eds). Proceedings of the 16th Nitrogen Workshop: Connecting different scales of nitrogen use in agriculture, Univ Milan, Turim, 367-368.

PEREIRA, José; MISSELBROOK, T.H.; CHADWICK, David; COUTINHO, João; TRINDADE, Henrique (2009) - Ammonia emissions from dairy cattle buildings and outdoor concrete yards under the Mediterranean conditions of NW Portugal. In: C. Grignani, M. Acutis, L. Zavattaro, L. Bechini, C. Bertora, P. Marino Gallina, D. Sacco (Eds). Proceedings of the 16th Nitrogen Workshop: Connecting different scales of nitrogen use in agriculture, Univ Milan, Turim, 193-194.

PIRRA A., BRÁS R., LUCAS M.S., PERES J.A. Tratamento de efluentes vinícolas por processos de coagulação/floculação química. Proceedings CD of 3rd International congress of energy and environment engineering and management (III CIIEM 2009), ISBN-13: 978-84-92669-15-8. Portalegre (Portugal). November 25-27, 2009, 4 pp.

PIRRA, A.; GUERRA, E.; PERES J.A.; "Bioremediação de efluentes da industria cárnica: optimização de processos", Proceedings CD of 3rd International Congress of Energy and Environmental Engineering and Management, ISBN-13: 978-84-92669-15-8. Portalegre (Portugal), November 25-27, 2009, 4 pp.

Short Abstracts

LUCAS M.S., MOSTEO R., MALDONADO M.I., MALATO S., PERES J.A. Solar treatment and detoxification of a winery wastewater in a CPC reactor. 1st International Edition - "Photocatalytic Products and Technologies Conference" PPTC'09. Guimarães, Portugal, 11th and 13th May 2009.

LUCAS M.S., Penela M., PERES J.A. Degradation of Reactive Black 5, Reactive Orange 16 and Acid Yellow 49 by advanced oxidation processes. 1st International Edition - "Photocatalytic Products and Technologies Conference" PPTC'09. Guimarães, Portugal, 11th and 13th May 2009.

LUCAS M.S., PENELA M., PERES J.A. Photochemical degradation of three commercial azo dyes used in the textile industry. 1st International Edition - "Photocatalytic Products and Technologies Conference" PPTC'09. Guimarães, Portugal, 11th and 13th May 2009.

LUCAS M.S., PERES J.A., Li Puma, G. Pilot-scale treatment of winery wastewater by ozonation and advanced oxidation. 1st International Workshop on Application of Redox Technologies in the Environment (Arte'2009), September 14-15, 2009, Istanbul-Turkey.

LUCAS M.S., PERES. J.A., LI PUMA G. Ozonation and advanced oxidation of winery wastewater in a pilot-scale bubble column reactor. 2nd European conference on environmental applications of advanced oxidation processes (EAAOP2). Cyprus, September 9 -11, 2009.

PACHECO, F.A.L.; Van der Weijden, C.H. (2009). Spring Residence Times: Role in Weathering rates. In: The 19th Goldschmidt Conference: Davos, Switzerland, 21-26 June 2009. Geochimica et Cosmochimica Acta, v. 73, no. 13S, Page A983.

Other publications National

Books

PERES J. A., Trabalhos Práticos em Química Ambiental, Série Didáctica, Ciências Aplicadas - nº 368, UTAD – Universidade de Trás-os-Montes e Alto Douro, Vila Real, 2009, ISBN: 978-972-669-905-7, 127 pp.

National journals

BRITO, Luis Miguel; MOURÃO, Isabel; TRINDADE, Henrique; COUTINHO, João (2009) - Produção de azoto mineral durante a compostagem de resíduos sólidos de chorume da pecuária leiteira intensiva. Revista de Ciências Agrárias 31 (1): 323-334.

Nogueira, J.; Seixas, V; Matos, C.; PERES, J.A. (2009) - Análise crítica e propostas de optimização de um sistema compacto de tratamento de águas residuais. Aplicação à ETAR de Folhadela (Vila Real), Indústria e Ambiente, 59, Novembro-Dezembro, p.9-13.

RIBEIRO, Henrique; VASCONCELOS, Ernesto; RAMOS, A.; COUTINHO, João (2009) – Avaliação do estado nutricional azotado de pés-mãe de Eucalyptus globulus Labill. spp. globulus com recurso a um medidor portátil de clorofila. Revista de Ciências Agrárias 31 (1): 40-49.

RIBEIRO, Henrique; VASCONCELOS; Ernesto, RAMOS, A.; COUTINHO, João (2009) – A fertilização azotada de pés-mãe de Eucalyptus globulus Labill.: feito no crescimento. Revista de Ciências Agrárias 31 (1): 50-62.

Proceedings in National Meetings

ANTUNES, Maria Cristina G., PINTO, S., BRAGA, Fernando G., 2009. Utilização da casca de pinheiro para a remoção de Bisfenol A de soluções aquosas. Proceedings do X congresso Nacional de Engenharia do Ambiente. I Congresso Lusófono de Engenharia do Ambiente. 1-2 Outubro, Faro, Portugal, pp 129-137.

BENTO, João; SILVA, Dinis Afonso; COUTINHO, João (2009) - Persistência da correcção de deficiências de boro em espécies florestais: aplicação de

Group Productivity

boro através de adubos com solubilidade reduzida. Actas do Congresso Florestal Nacional, Ponta Delgada, 289-293.

BRAGA, Fernando G., GUEDES, M., ANTUNES, Maria Cristina G., 2009. Aplicação da permuta iónica ao processamento de efluentes produzidos por destilarias vínicas. Proceedings do X congresso Nacional de Engenharia do Ambiente. I Congresso Lusófono de Engenharia do Ambiente.1-2 Outubro, Faro, Portugal, pp 138-148.

Extended abstracts

COUTINHO, João (2009) – Ciclagem do azoto e carbono no solo e a aplicação de materiais orgânicos: fluxos de mineralização (Conferência plenária). Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 66-67.

Short abstracts

BRITO, Luís Miguel; AMARO, A.L.; MOURÃO, Isabel; COUTINHO, João (2009) – Evolução das características físico-químicas e dinâmica dos nutrientes durante a compostagem da fracção sólida do chorume. Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 90.

CARNEIRO, João; COUTINHO, João; TRINDADE, Henrique (2009) – Perdas de azoto na forma de N2O resultantes da utilização agrícola de diferentes resíduos orgânicos. Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 78.

COUTINHO, João; FIDALGO, Paula; LAGOA, Rui; ALVES, Ricardo; CABRAL, Fernanda (2009) – Decomposição dos compostados aplicados ao solo: efeito da sua estabilidade. Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 95.

FANGUEIRO, David; VASCONCELOS, Ernesto; CABRAL, Fernanda; RIBEIRO, Henrique; COUTINHO, João (2009) – Tratamento de chorumes de porco por acidificação e separação: efeito na mineralização do azoto e carbono após incorporação ao solo. Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 71.

MENDES, Susana; FANGUEIRO, David; CABRAL, Fernanda; COUTINHO, João, (2009) – Previsão do azoto mineralizável e disponível de diferentes fracções de chorume de suíno incorporadas ao solo: método de incubação anaeróbia-extracção. Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 74.

MOURÃO, Isabel; BRITO, Luís Miguel; COUTINHO, João (2009) – Influência da dose e do momento da aplicação ao solo de um compostado no crescimento da cebola no modo de produção biológico. Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 106.

PERDIGÃO, Adelaide; COUTINHO, João; MOREIRA, Nuno (2009) – Potencialidade de leguminosas forrageiras anuais como fonte de azoto em agricultura biológica. Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 70.

RAIMUNDO, Fernando; MARTINS, Afonso; DUARTE, J.; COUTINHO, João; FARROPAS, L.; MANO, Raquel; LOURENÇO, M.; ARANHA, José; MADEIRA, Manuel (2009) – A fertilidade dos solos florestais de Portugal Continental e relações com factores ambientais. Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 93.

ROBOREDO, Marta; COUTINHO, João (2009) – A utilização de membranas de troca aniónica na construção de isotermas de desadsorção do fósforo. Livro de Resumos do Encontro Anual da Ciência do Solo, Univ Algarve, Faro, pp. 87.

Santos C., LUCAS M.S., PERES J.A., Sampaio A. (2009) - Tratamento de efluentes vinícolas por combinação de processos químicos e biológicos. 3as Jornadas de Biologia na UTAD. Vila Real, 21 e 22 Outubro.

CARVALHO, G.J.P.; PACHECO, F.A.L. (2009). Análise da vulnerabilidade à contaminação das águas subterrâneas na bacia hidrográfica do rio Sordo (Vila Real) pelo método fuzzy-DRASTIC. In: 1º Seminário sobre Gestão de Bacias Hidrográficas subordinado ao tema: As Regiões Hidrográficas do Norte e as Perspectivas Futuras de Gestão", FEUP, 6 e 7 de Maio de 2009.

CAETANO, C.A.R.; PACHECO, F.A.L. (2009). Caracterização de bacias hidrográficas para fins de aproveitamento hídrico no concelho de Torre de Moncorvo utilizando os modelos ARCHYDRO e ARCSWAT. In: 1º Seminario sobre Gestão de Bacias Hidrográficas subordinado ao tema: As Regiões Hidrográficas do Norte e as Perspectivas Futuras de Gestão", FEUP, 6 e 7 de Maio de 2009.

ALENCOÃO, A.M.P.; PACHECO, F.A.L. (2009). Estimativa de parâmetros hidrológicos à escala da bacia hidrográfica: dois modelos, um caso em estudo. In: 1º Seminario sobre Gestão de Bacias Hidrográficas subordinado ao tema: As Regiões Hidrográficas do Norte e as Perspectivas Futuras de Gestão", FEUP, 6 e 7 de Maio de 2009.

Master and Ph.D. thesis completed

PhD thesis

LUCAS, Marco Paulo Gomes Sousa (2009). Aplicação de Processos de Oxidação Avançada ao Tratamento de Águas Residuais. Tese de doutoramento. UTAD, Vila Real, 2009. Orientação: José Alcides Peres.

Master thesis

SANTOS, Cátia Filipa Pinheiro dos (2009). Tratamento de efluentes vinícolas por combinação de processos químicos e biológicos. Mestrado em Engenharia do Ambiente (2º ciclo). UTAD, Vila Real. Orientação: José Alcides Peres, em colaboração com a Profª Ana Cristina Sampaio, DeBA).

CAETANO, Carla Alexandra Rodrigues (2009). Caracterização Hidrológica de Bacias Hidrográficas Utilizando Sistemas de Informação Geográfica na Região de Trás-os-Montes e Alto Douro. Mestrado (pré-Bolonha) em Sistemas de Informação Geográfica. UTAD, Vila Real. Orientação: Fernando Pacheco.

CARVALHO, Gonçalo Jorge Pires de (2009). Vulnerabilidade à Contaminação das Águas Subterrâneas na Bacia Hidrográfica do Rio Sordo: Comparação de Modelos Baseados no Método DRASTIC. Mestrado (pré-Bolonha) em Sistemas de Informação Geográfica. UTAD, Vila Real. Orientação: Fernando Pacheco.

PERDIGÃO, Maria Adelaide Homem (2009) - Potencialidade de Leguminosas Forrageiras Anuais como Fonte de Azoto em Agricultura Biológica. Mestrado em Engenharia Agronómica. Orientação: Nuno Moreira e João Coutinho.

Group Productivity

PINTO, Sandra Isabel Portela (2009) – Remoção de poluentes orgânicos da água utilizando adsorventes naturais, UTAD, Vila Real. Orientação: Maria Cristina Antunes e Fernando Glenadel Braga.

Patents/propotypes

Conceded patents:

CLARO J., VALENTE A., ROSA PIRES A.- "Processo de aglomeração de partículas dos sectores da madeira e da cortiça". Portuguese patent n.º103 693, UTAD. Conceded at July 28 of 2009.

CLARO J., VALENTE A., ROSA PIRES A. – "Processo de aglomeração de fibras de madeira para a produção de placas ou painéis de aglomerado". Portuguese patent n.º103 702, UTAD. Conceded at June 08 of 2009.

CLARO J., VALENTE A., ROSA PIRES A. - "Processo de produção de biomassa a partir de resíduos e efluentes industriais em particular dos sectores da madeira, cortiça e celulose".

Portuguese patent n. º103 739, UTAD. Conceded at June 07 of 2009.

LUCAS M.S., PERES J.A., Amaral C., Sampaio A., Dias A.A. Processo biológico aeróbio de tratamento de efluentes agro-industriais com elevado teor em compostos aromáticos baseado na aplicação de microrganismos da espécie Candida oleophila. Portuguese patent nº 103 738, UTAD. Conceded at August 8, 2009.

Organization of conferences

IV Jornadas do Ambiente, 19 de Junho 2009, Escola EB2,3 de Vila Pouca de Aguiar. Member of Organization Committee: Fernando Pacheco.

16th Nitrogen Workshop, João Coutinho, co-chairman of session: "Manure processing for sustainable nitrogen management". 28/6 – 1/7/2009, Univ. Milan, Turim.

Encontro Anual da Ciência do Solo, Univ Algarve, Faro, 8–10 Julho 2009. Member of Scientific Committee: João Coutinho

PPTC'09 - Photocatalytic Products and Technologies Conference, Universidade do Minho, Guimarães, 11-13 Maio 2009. Member of Scientific Committee: José Alcides Peres.

Industry contract research

Desenvolvimento de Novos Fertilizantes para a Agricultura. Projecto em parceria com o ISA – Departamento de Química Agrícola e Ambiental e com a empresa CUF, Adubos de Portugal. Montante Anual de Financiamento: 10000 €

BioCombus – Recovery of Wastes as Bio Fuel - a process for the treatment and recovery of wastes and effluents from olive oil production units, Cooperativa Agrícola dos Olivicultores de Murça, FP7 Nº 3483, PI: J.C. Claro. 1 168 574 €. (10/2008 - 09/2011).

Winery wastewater treatment by a combination of chemical and biological processes. Supported by Águas de Trás-os-Montes e Alto Douro, 24 000 €. PI: J. A. Peres (05/2006 - 04/2010).

Modelling nitrogen mineralization in Eucalyptus globulus stands, in collaboration with RAIZ, Instituto de Investigação da Floresta e do Papel. 10 000 €/year (2009)

Internationalization

.Training periods and collaborative publications with:

- Department of Chemical and Environmental Engineering, University of Nottingham (England) – Prof. Gianluca Li Puma;

- Plataforma Solar de Almeria – CIEMAT (Spain) – Dr. Sixto Malato;

- Departamento de Ingeniería Química y Química Física, Universidad de Extremadura, Badajoz (Spain) – Prof. Jesús Beltran-Heredia e Prof Joaquín Domínguez.

Future Research

Objectives

1. Study different treatment processes of winery wastewaters (a great problem in Douro region) by a combined treatment involving biological processes and Fenton's reagent and by AOPs with ozone, ozone/UV and ozone/UV/H2O2. We also will study the reaction of phenolic acids typically presents in agro-industrial wastewaters with Fenton-generated hydroxyl radicals and will deduce the Hammett correlation. It will be evaluated the photochemical degradation of personal care products, particularly parabens, from water by AOPs processes namely UV, UV/H2O2, Fenton and photo-Fenton processes. Finally, we will study the decolouration of orange II solutions by TiO2 and ZnO active layers screen-printed on ceramic tiles under UV radiation.

Investigate the adsorption potential of low-cost biosorbents: brown algae (in different ionic forms, e.g. Ca, K, Na, Mg) for the removal of toxic metals present in mining and industrial effluents using a biosorption process.

Collection and pre-treatment of the selected brown marine macro-algae; Physico-chemical and ecotoxicological characterization of the metal bearing effluents; biosorption process (kinetic and equilibrium studies in batch mode) of metal ions from contaminated effluents will be studied using the selected biosorbents; desorption and regenerations studies.

2. Compare the adsorption capacity of alternative adsorbents, such as, agricultural by-products, resins and zeolites for removal emerging organic contaminants (pharmaceutically compounds and endocrine disrupting chemical) from aqueous matrices.

3. Study the application of higher plants as biomarkers for organic pollutants:

• Identification of higher plants with potential capacity to accumulate atmospheric organics pollutants

Future Research

• Selection of organic pollutants to be studied, ideally from different classes, according to their environmental relevance and its octanol-water partition coefficients

• Validation of environmental friendly analytical methodologies to perform the extraction and quantification of pollutants under study.

4. Technology transference based on patent process. Recovery of shoe industry wastes, namely leather dust. Composite boards based on cork and ceramic waste particles.

5. Study the weathering process of fractured rocks, at the small watershed scale, in the framework of isotope geochemistry.

6. - Test organic amendments with dissimilar characteristics in order to compare different C and N turnover patterns;

- To study boron slow release fertilizers in field under Eucalyptus globulus stands.

- To study the composting process and agronomic value of composts derived from on-farm residues.

To study phosphorus dynamics in soils amended with animal manures and to create an evaluation tool to identify the risk of P losses to the surface water bodies.

To apply a phosphorus desorption method based on the use of anion exchange resins to different agricultural soils. Desorption isotherms allow a better understanding of the reversibility of soil phosphorus, being particularly useful in predicting crops needs and environmental risks.

Phosphorus bioavailability in soils derived from volcanic material with laboratory methods and pot trials. In collaboration with U. Açores and SRAP

Funding, source, dates

BioCombus – Recovery of Wastes as Bio Fuel - a process for the treatment and recovery of wastes and effluents from olive oil production units, FP7 Nº 3483, 1 168 574 €. (10/2008 - 09/2011).

Winery wastewater treatment by a combination of chemical and biological processes. Supported by Águas de Trás-os-Montes e Alto Douro (05/2006 - 04/2010), 24 000 €. J.A. Peres.

SUVIDUR, Viticulture sustainability in Douro Valley, INTERREG/POCTEP411 433 €

Development of new fertilizers to agriculture, CUF, Adubos de Portugal. 10 000 €/year.

Modeling nitrogen mineralization in Eucalyptus globulus stands, in collaboration with RAIZ, Instituto de Investigação da Floresta e do Papel. 10 000 €/year

Boron slow release fertilsers, in collaboration with Borax Inc., 5000 €/year

Pending:

Ecovinis - Winery wastewater treatment by combined anaerobic and solar AOP processes, PTDC/AGR-AAM/101558/2008, 91 599 €.

Decontamination and decolourisation of inorganic agents by photocatalysis with layered supported semiconductors deposited in common substrates by simple techniques, PTDC/AAC-AMB/101010/2008, 57 480 €.

Effect of phytochemicals on the organic residues transformation and on key processes of the C and N cycles. PTDC/AGR-AAM/102006/2008, €125 680

Emissões gasosas medidas em campos regados de arroz produzido em dois solos diferentes, em Portugal, por efeito das práticas culturais, do clima e do aumento da concentração de CO2 na atmosfera. FCT: PTDC/AGR-AAM/102529/2008, 45 360 € (2010-2012)

Greenhouse gases emissions from rice fields in two Portuguese soil conditions. FCT: PTDC/AGR-AAM/102529/2008. 45 360 €

Assessment of phosphorus bioavailability from animal manures applied to Portuguese soils and site vulnerability to phosphorus", PTDC/AGR-PRO/112127/2009, 114 561 €.