

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. More recently the staff includes 3 investigators from Ciência programme. Since its creation the Unit has had a slowly but consistent growing in members. In 2010 the CQVR increased from 23 to 28 PhD full members.

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 2010 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 (10 PhDs), Materials Chemistry (7 PhDs) and Environmental Chemistry (11 PhDs).

In 2010 the CQVR members and the Rector of UTAD approved a new regulation for the CQVR that was published in "Diario da Republica" in the 23 of July 2010. The link to the text is http://home.utad.pt/~cqvr/Regulamento_do_CQVR_Diario_da_Republica_23_Julho_2010.pdf.

In this regulation 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 Advisory Board.

Following to the approval of the regulations we promoted elections for the Direction and for the Principal Investigators. The elected members are:

Director: Pedro Manuel de Melo Bandeira Tavares

Vice-Directors: José Alcides Silvestre Peres; Maria Cristina Fialho Oliveira

PI: Paulo Coelho; Verónica Zea Bermudez; José Alcides Silvestre Peres

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. We want to emphasize two QREN projects with near 2MEuros, and 4 new FCT projects that started in 2010.

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 applied research on Chemistry topics ;
2. to provide a modern and high level of scientific research training;
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:

- Synthesis and structural characterization of organic compounds with applications in photochromic devices, photodynamic therapy, affinity chromatography and pharmaceuticals.
- 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 and kinetic studies of catalysts: new metal complexes covalent anchored on the surface of inorganic materials to be used as hybrid organic – inorganic catalysts; nanoparticles doped with noble metals.
- 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 2010

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, in particular the review articles. 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 scientific production of this unit increased in the last year. The objective of publishing in high impact SCI journals (IF>2) was successfully achieved. In 2010 we have submitted 3 new patents, published 50 papers in SCI peer-review journals, 2 book chapter and 32 conference proceedings. In addition, more than 60 oral and poster communications were presented in national and international scientific meetings.

2. This performance was possible due to the dynamism of the team. In 2010 we obtained approval in 4 new FCT projects, with the lead of CQVR members, and another 8 FCT projects with the lead of other institutions. These projects will start in 2011.
3. The CQVR members, as principal investigators, submitted 5 new projects in FCT/2010 call, currently under evaluation.
4. A large QREN project was approved, with a total of 565 751 €, to investigate "Confitage techniques of fruits and vegetables without sucrose". This project is also supported by NUTRIDOURO, a Portuguese food company.
5. As always, particular attention was paid to collaboration/interaction with industry. 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.
6. Extension activities, concerning water and wastewater analysis for local councils and other public bodies were continued.
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. In 2010 the CQVR members and the Rector of UTAD approved a new regulation for the CQVR that was published in "Diario da Republica" in the 23 of July 2010. The link to the text is http://home.utad.pt/~cqvr/Regulamento_do_CQVR_Diario_da_Republica_23_Julho_2010.pdf.
9. Under the new regulation, an advisory board was named, consisting of Professors Carlos Costa, Paulo Ferreira and Mark Heron. Their reports are available at http://home.utad.pt/~cqvr/Consultive_Council
10. In 2010 the CQVR, in collaboration with the Chemistry Department and the Biological Department submitted to A3ES (Agência de Avaliação e Acreditação do Ensino Superior) a new PhD programme "Chemical and Biological Sciences".

Activities

Integrative/multidisciplinary activities during the year of 2010

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 photocytotoxicity 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, Lisbon, Porto) and foreign Universities (Lille, Marseille, Paris VII, Toulouse, Katholieke, Leuven, Nottingham, Almeria).
- 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).
- 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 , ^{13}C and ^{29}Si NMR, FEG/SEM, AFM); Applied Physics Dep. of the Chalmers Univ. of 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 2010

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.

6ª Olimpíadas de Química Júnior (6 th Junior Chemistry Olympics), 17 April 2010. Centro de Química - Vila Real and Chemistry Department. An event with 51 teams, 21 schools and 153 students.

BRAGA F. - A Química que falta descobrir. Acção de divulgação no Colégio Nossa Senhora da Boavista, Vila Real, 05 de Março de 2010.

PERES J.A. - A água: um bem essencial que devemos respeitar. Comemorações do Dia Mundial da Água, Escola Secundária/3 de Vila Nova de Paiva (Viseu), 26 de Março 2010.

PIRRA, A. Organização do Fórum e apresentação de comunicação intitulada "Caminhos do projecto Ecocidadania: Fossas sépticas, água e energia", Fórum Biodiversidade de SeVer, 15 de Junho 2010, Centro de Artes de Sever do Vouga (Fórum final do projecto Ecocidadania).

Gestão operacional de uma rede interlaboratorial ibérica para análise de solos e materiais orgânicos (plantas e correctivos/resíduos orgânicos). Nº de laboratórios participantes no final de 2010: 74 membros de Portugal e Espanha, Laboratórios de Investigação ou de Prestação de Serviços, Laboratórios Oficiais e Particulares. A rede interlaboratorial é reconhecida como Comissão Permanente da Sociedade Portuguesa de Ciência do Solo. Responsável na UTAD: João Coutinho.

Funding

	2008	2009	2010
LA FCT	0,00	0,00	0,00
Units FCT	80.000,00	90.749,00	90.750,00
Projects FCT	48.073,00	119.403,00	205.927,00
Other (National)	0,00	10.600,00	73.414,00
Other (International)	0,00	137.144,00	137.144,00
National Industry	415.525,00	415.525,00	645.442,00
International Industry	0,00	0,00	0,00
	543.598,00	773.421,00	1.152.677,00

General Indicators

	2006	2007	2008	2009	2010	Total
No. of Researchers Proposed	0,00	0,00	0,00	0,00	0,00	0,00
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	2,00	1,00	0,00	3,00
No. of Researchers integrated with PhD	16,00	20,00	23,00	23,00	28,00	
Training Masters (Master thesis completed)	2,00	1,00	3,00	10,00	0,00	16,00
Training PhDs (PhD thesis completed)	0,00	2,00	2,00	2,00	0,00	6,00

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

a) FCT:

Designing ultra-fine textured microstructures by laser floating zone - LaFlorZone, PTDC/CTM/66195/2006, P.Tavares, CQVR: 10 800 €. 2008/11.

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

Multiferroicos e magnetoeléctricos para spintrónica: barreiras e interfaces PTDC/CTM/099415/2008, P.Tavares, CQVR: 29.232€. 2010/12.

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 € (2008/2010)

Híbridos orgânicos-inorgânicos com propriedades de emissão optimizadas para aplicação na nova geração de comunicações ópticas. PTDC/CTM/101324/2008. CQ-VR: 36182 € (2010-2012)

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

b) Other.

Materiais híbridos multifuncionais: nanoestruturação por auto-organização e por reconhecimento molecular. Programa Pessoa (Departamento das Relações Europeias, Bilaterais e Multilaterais da FCT)/Programme Hubert Curien (Égide) Ref^a 441.00. CQ-VR: 7200 € (2009-2010)

Objectives & Achievements

Objectives

Organic/inorganic hybrid materials

To develop 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. To graft to the inorganic skeleton or simply add several ionic liquids with the goal of enhancing the ionic conductivity. Applications in the fields of advanced solid state batteries, electrochromic devices, optics, and medicine were envisaged.

To develop 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 carry out 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 were foreseen.

Ceramic materials

The multiferroic properties of ceramic systems like $\text{Bi}_{1-x}\text{La}_x\text{Fe}_{1-y}\text{Mn}_y\text{O}_3$, $\text{Re}_1\text{Re}_2\text{MnO}_3$ ($\text{Re}_1=\text{Eu, Gd, Tb, Dy}$; $\text{Re}_2=\text{Y, Ho, Lu}$) will continue to be evaluated. We intend to produce thin films by Pulsed Laser Deposition and by RF-sputtering. To do this, high quality targets needed to be produced. A laboratory to measure film and bulk ceramic properties like leakage currents, polarizations or dielectric constants will continue to be installed in collaboration with Physics Department of UTAD.

We will continue the production of fibers and monocrystals by Laser Floating Zone of the $\text{Re}_1\text{Re}_2\text{MnO}_3$ ($\text{Re}_1=\text{Eu, Gd, Tb, Dy}$; $\text{Re}_2=\text{Y, Ho, Lu}$) systems.

Catalysts materials

Different systems will be analysed such as metal complexes, magnetic $\gamma\text{-Fe}_2\text{O}_3@\text{SiO}_2$ nanoparticles and supported metal nanoparticles. We will continue the synthesis and characterization of alkoxysilane pentacoordinate oxovanadium(IV) complexes. These metal complexes will be anchored on SiO_2 and Al_2O_3 as hybrid catalysts. Well characterized final catalysts will be applied for the hydro-isomerization and oxidation of hydrocarbons in micro batch reactor. Nobel metal/ TiO_2 and CeO_2/Au nanoparticles will be tested as catalysts in the oxidation of CO.

In electrocatalysts materials the development of fuel cells is dependent on the improvement of the gas diffusion electrodes (GDE). Their catalytic properties and design are the key to control the reaction kinetics, mass transport and to avoid the poisoning of the catalyst surface during the fuel cell operation. In the last year a new architecture of gas diffusion electrode has been developed which enables the electronic contact with carbon substrate and the preferential location of the catalyst nearby the membrane electrolyte, resulting in a higher efficient catalyst. It is now our goal to apply the new electrode design to novel electrode materials to work as anode and/or cathode of low temperature fuel cells. The novel materials will be prepared as metal-non metal alloys, because these materials are known to be much more resistant to corrosion, and therefore to sintering phenomena, than bimetallic alloys.

Main Achievements

Organic/inorganic hybrid materials

Prototype ECDs incorporating electrolytes based on (POE)/siloxane hybrid networks doped with lithium tetrafluoroborate or PCL/siloxane hybrid networks doped with potassium triflate or mixed Li^+ and Eu^{3+} triflate salts, were produced. The thermal, morphological, structural and electrochemical features of the electrolytes were studied. The electro-optical behaviour of the devices was characterized. POE/siloxane hybrid electrolytes doped with magnesium triflate ($\text{Mg}(\text{CF}_3\text{SO}_3)_2$) with foreseen application in batteries were studied.

The role of lanthanide ions, solvent polarity and length of the alkyl-based side spacers on the structure, morphology and luminescent features of bridged silsesquioxanes incorporating central alkyl-based spacers of variable length and synthesized by means of sol-gel reactions and self-directed assembly were investigated.

The structure, the order/disorder phase transitions and the optical memory effect of lamellar bilayer alkylsilanes were examined.

The influence of several polymers on the growth habit of calcium carbonate polymorphs was investigated.

Ceramic Materials

The crystal structure, morphology, dielectric and magnetic properties, temperature dependence of the electric polarization of $\text{Eu}_{1-x}\text{Y}_x\text{MnO}_3$ ceramics, synthesized by urea sol-gel combustion method were investigated. Temperature dependence of the structural parameters was investigated using synchrotron radiation. A significant magnetoelastic coupling is revealed by anomalies observed in lattice parameters at the magnetic phase transitions, apparent also in both Mn-O bond lengths and Mn-O1-Mn bond angle and involving rotations of the MnO_6 octahedra.

The hexagonal $\text{Y}_{1-x}\text{Eu}_x\text{MnO}_3$ ceramics were studied using IR and THz spectroscopies in the temperature range between 5 and 900 K.

Catalysts Materials

Superparamagnetic $\gamma\text{-Fe}_2\text{O}_3$ was synthesized by the co-precipitation method, coated with two silica shells, and applied as support for the immobilization of $[\text{VO}(\text{acac})_2]$. The catalytic performance in the epoxidation of geraniol, with easy recovery by magnetic separation, was demonstrated.

We have synthesized and characterized trimethoxysilane pentacoordinate V(IV), Cu(II) and Co(II) complexes, scorpionate Fe complexes and macrocyclic. These complexes are anchored into inorganic matrix via covalent bond as new supported hybrid catalysts. Remarkable catalytic effects with molecular O_2 were observed for cyclohexane and n-hexane oxidation.

CeO_2 nanoparticles were prepared by a solvothermal method. Au was loaded onto the obtained ceria supports by a double impregnation (DIM) method. The effect of chloride on the sinterization of Au/ CeO_2 catalysts was investigated. Noble metal catalysts (Pt, Pd, Ir, Rh and Au) were supported on TiO_2 . These catalysts were tested in the oxidation of CO, ethanol and toluene.

In electrocatalyst materials:

Cathode material:

The Pd-P catalysts were directly deposited on a commercial gas diffusion layer porous carbon paper with teflon, to form the catalyzed gas diffusion electrode by electroless deposition method. Their electrochemical activities for the oxygen reduction reaction were determined in sulfuric acid solution with and without methanol. The catalysts were characterized by AAS, SEM/EDS, TEM, XRD and XPS.

Compared to pure Pd and Pt/C, results showed that the ORR activity of Pd-P alloy was highest and its methanol tolerance was better than Pt/C catalyst.

The pure Pd electrodes were also tested as cathodes of PEMFCs. For comparison purposes, MEAs with Pt catalyst in their cathodes were also prepared.

Promising results have been obtained, which have shown that it is possible to use Pd-catalyzed electrodes prepared by electroless deposition as oxygen diffusion cathodes in PEMFCs.

Anode material:

Pd-Ag alloys containing different amounts of Ag were prepared in order to evaluate their catalytic activity towards the ethanol oxidation (EOR) and oxygen reduction (ORR) reactions. A sequential electroless deposition of Ag and Pd on a stainless steel disc, followed by annealing at 650 C under Ar stream, was used as the alloy electrode deposition process.

From half-cell measurements, it was found that alloying Pd with Ag leads to an increases of the ORR and EOR kinetics, relative to Pd. Among the alloys under study, the 21 % at. Ag content alloy presents the highest catalytic activity for the EOR and the lowest Ag content alloy (8 % at Ag)

shows the highest ORR activity. Moreover, it was found that the selectivity of Pd-Ag alloys towards ORR is sustained when ethanol is present in the electrolyte.

Group Productivity

Publications in peer review Journals

1. AGOSTINHO MOREIRA J., ALMEIDA A., FERREIRA W. S., TAVARES P.B., VILELA S.M.F. (2010) - Coupling between phonons and magnetic excitations in orthorhombic $\text{Eu}_{1-x}\text{Y}_x\text{MnO}_3$, *Physical Review B* 81, 054447. (IF 2009 = 3.475)
2. AGOSTINHO MOREIRA J., ALMEIDA A., FERREIRA W.S., CHAVES M.R., VILELA S.M.F., TAVARES P.B., KUNDYS B., RANJITH R., PRELLIER W., (2010) - Effect of the external fields on the polar and dielectric properties of $\text{Eu}_0.8\text{Y}_0.2\text{MnO}_3$, *Journal of Applied Physics* 107 024108. (IF 2009 = 2.072)
3. CARABINEIRO S.A.C., SILVA A.M, DRAŽIĆ G., TAVARES P. B., FIGUEIREDO J.L. (2010) - Effect of chloride on the sinterization of Au/CeO₂ catalysts, *Catalysis Today* 154, 293-302. (IF 2009 = 3.526)
4. CARABINEIRO S.A.C., SILVA A.M.T., DRAZIC G., TAVARES P.B, FIGUEIREDO J.L. (2010) - Gold Nanoparticles on Ceria Supports for the Oxidation of Carbon Monoxide, *Catalysis Today* 154, 21-30. (IF 2009 = 3.526)
5. FERREIRA R. A. S., OLIVEIRA D.C., MAIA L.O., VICENTE C.M.S., ANDRÉ P. S., DE ZEA BERMUDEZ V., RIBEIRO S.J.L., CARLOS L.D., Enhanced photoluminescence features of Eu^{3+} -modified di-ureasil-zirconium oxocluster organic-inorganic hybrids, *Optical Materials* 32 (12) pp: 1587-1591. (IF 2009 = 1.728)
6. GOIANA V., KAMBA S., KADLEC C., NUZHNYI D., KUZEL P., AGOSTINHO MOREIRA J., ALMEIDA A., TAVARES P.B. (2010) - THz and infrared studies of multiferroic hexagonal $\text{Y}_{1-x}\text{Eu}_x\text{MnO}_3$ ($x=0-0.2$) ceramics, *Phase Transitions* 83 (10-11) pp.931-941. (IF 2009 = 0.935)
7. GONÇALVES M. C., DE ZEA BERMUDEZ V., SILVA M. M., SMITH M. J., MORALES E., SÁ FERREIRA R. A., CARLOS L. D. (2010) - Structure, thermal properties, conductivity and electrochemical stability of di-urethanesil hybrids doped with LiCF_3SO_3 . *Ionics* 16 193-201. (IF 2009 = 0.899)
8. GOPAL S. M., ANIL K., SUMAN M., TAVARES P.B. (2010) - Novel alkoxy silane pentacoordinate $\text{O}=\text{V}(\text{IV})$ complexes as supported catalysts for cyclohexane oxidation with dioxygen, *Applied Catalysis A: General* 384, 136-146. (IF 2009 = 3.564)
9. MOREIRA J.A., ALMEIDA A., FERREIRA W. S., ARAÚJO J. P., PEREIRA A. M., CHAVES M. R., COSTA M.M.R., KHOMCHENKO V.A., KREISEL J., CHERNYSHOV D., VILELA S.M.F., TAVARES P.B. (2010) - Strong magnetoelastic coupling in orthorhombic $\text{Eu}_{1-x}\text{Y}_x\text{MnO}_3$ manganite, *Physical Review B* 82, 094418 (1-9). (IF 2009 = 3,475)
10. MOREIRA J.A., ALMEIDA A., FERREIRA W.S., CHAVES M.R., ARAÚJO J.P., PEREIRA A.M., VILELA S.M.F., TAVARES P.B. (2010) - Polar properties and phase sequence in $\text{Eu}_0.8\text{Y}_0.2\text{MnO}_3$, *Journal of Physics - Condensed Matter* 22 (12) 125901. (IF 2009 = 1.964)
11. MOREIRA J.A.; ALMEIDA A., FERREIRA W.S., CHAVES M.R., OLIVEIRA J., DA SILVA J. M., SÁ MARIA, VILELA S.M.F., TAVARES P.B. (2010) - Structure and physical properties of $\text{Eu}_0.8\text{Y}_0.2\text{MnO}_3$ ceramics, *Journal of Electroceramics* 25, 203-211. (IF 2009 = 1.012)
12. NOBRE S. S., CATTOËN X., FERREIRA R. A. S., CARCEL C., DE ZEA BERMUDEZ V., WONG CHI MAN M., CARLOS L. D. (2010) - Eu^{3+} -Assisted Short-Range Ordering of Photoluminescent Bridged Silsesquioxanes, *Chemistry of Materials* 22 (12), 3599-3609. (IF 2009 = 5.368)

13. NOBRE S. S., FERREIRA R. A. S., CATTOËN X., BENYAHYA S., TAILLEFER M., DE ZEA BERMUDEZ V., WONG CHI MAN M., CARLOS L. D. (2010) - Lanthanide-Containing 2,2'-Bipyridine-urea Bridged Urea Cross-linked Polysilsequioxanes, *Spectroscopy Letters* 43, 321-33 (IF 2009 = 0.585)
14. NUNES S.C., PLANELLES-ARAGO J., FERREIRA R.A.S., CARLOS L.D., DE ZEA BERMUDEZ V., (2010) Eu-III-Doping of Lamellar Bilayer and Amorphous Mono-Amide Cross-Linked Alkyl/Siloxane Hybrids, *European Journal of Inorganic Chemistry*, 18 pp: 2688-2699. (IF 2009 = 3.101)
15. PEREIRA C., PEREIRA A. M., QUARESMA P., TAVARES P. B., PEREIRA E., ARAÚJO J. P., FREIRE C. (2010) - Superparamagnetic γ -Fe₂O₃@SiO₂ nanoparticles: a novel support for the immobilization of [VO(acac)₂], *Dalton Transactions* 39, 2842–2854. (IF 2009 = 4.081)
16. REGO R., OLIVEIRA C., VELÁZQUEZ A., CABOT P.-L. (2010) - A new route to prepare carbon paper-supported Pd catalyst for oxygen reduction reaction. *Electrochemistry Communications* 12, 745-748. (IF 2009 =4.243)
17. SANTOS V.P., CARABINEIRO S.A.C., TAVARES P.B., PEREIRA M.F.R., ÓRFÃO J.J.M., FIGUEIREDO J. L. (2010) - Oxidation of CO, ethanol and toluene over TiO₂ supported noble metal catalysts, *Applied Catalysis B: Environmental* 99, 198-205. (IF 2009 = 5.252)
18. TEIXEIRA J. C. S., FERNANDES M., DE ZEA BERMUDEZ V., BARBOSA P. C., RODRIGUES L., SILVA M. M., SMITH M. J. (2010) - Mg²⁺-doped poly(ϵ -caprolactone)/siloxane biohybrid electrolytes. *Electrochimica Acta* 55 1328-1332. (IF 2009 = 3.325)
19. VILELA S. M. F., ALMEIDA PAZ F.A., TOMÉ J. P. C., DE ZEA BERMUDEZ V., CAVALEIRO J. A. S., ROCHA J. (2010) - Trimethyl 2,2',2''-[1,3,5-triazine-2,4,6-triyltris(azanediyl)]triacetate, *Acta Crystallographica Section E*, 66., O3243–O3244. (IF 2009 = 0.411)

Other international publications

Books: (1)

DE ZEA BERMUDEZ V., SILVA M. M. (2010) - Lithium-doped hybrid polymer electrolytes, In *Polymer Electrolytes: Fundamentals and Applications*, D. Santos and C. Sequeira Eds., Woodhead Publishing Limited, Cambridge, Chapter 5. ISBN 1 84569 772 3.

Proceedings or extended abstracts (7)

PINTO J., VARUM H., CRUZ, D., SOUSA D., MORAIS P., TAVARES P., LOUSADA J., SILVA P., VIEIRA J. (2010) - Characterization of Traditional Tabique Constructions in Douro North Valley Region - *Journal WSEAS Transactions on Environment and Development*, ISSN 1790-5079, Issue 2, Vol. 6, February 2010, 105-114.

SILVA B., CORREIA J., NUNES F.; TAVARES P.B., VARUM H., PINTO J. (2010) - Bird Nest Construction: Lessons for Building with Earth - *Journal WSEAS Transactions on Environment and Development*, ISSN 1790-5079, Issue 2, Vol. 6, February 2010, 95-104.

CEPEDA A. M., LOUSADA J., VIEIRA J., VARUM H., TAVARES P.B., FERNANDES L., PINTO J. (2010) – Estudo do material terra aplicado na construção de tabique existente no Alto Tâmega – Resumo Alargado in *Terra em Seminário 2010, 6º Seminário Arquitectura de Terra em Portugal e 9º Seminário Ibero-Americano de Arquitectura e Construção com Terra*. ARGUMENTUM. Editores: Maria Fernandes, Mariana Correia, Filipe Jorge. 1ª Edição – Fevereiro de 2010. ISBN: 978-972-8479-67-1. pgs. 160-162.

CEPEDA A. M., LOUSADA J., VIEIRA J., PINTO J., FERNANDES L., TAVARES P.B., SILVA P., VARUM H. (2010) - Tabique construction in Alto Tâmega. Resumo Alargado in *CD-ROM of full papers of the 1st International Conference on Structures and Architecture (ICSA2010)*. Ed. Paulo Cruz. CRC Press, Taylor & Francis Group. London. ISBN 978-0-415-49249-2. pgs. 1403-1410.

PINTO J., VARUM H., CEPEDA A., TAVARES P., LOUSADA J., SILVA P., VIEIRA J. (2010). Study of the traditional tabique constructions in the Alto Tâmega region. In The Sustainable World. Editor: C.A: Brebbia. WIT Press 2011. WIT eLibrary. British Library - ISBN: 978-1-84564-504-5 - ISSN: 1746-448X (print) - ISSN: 1743-3541 (on-line). pgs. 299-307.

MURTA A., PINTO J., VARUM H., GUEDES J., LOUSADA J., TAVARES P. (2010) – Survey on the main defects in ancient buildings constructed mainly with natural raw materials - Portugal SB10, Sustainable Building, Affordable to All, Low Cost Sustainable Solutions. Edited by: Bragança L.; Pinheiro M.; Mateus R.; Amoêda R.; Almeida M.; Mendonça P.; Cunha A.; Dias A.; Farinha F.; Gervásio H.; Brito J.; Guedes M.; Ferreira V., 1st edition: March 2010, ISBN 978-989-96543-1-0, Chapter 5: Monitoring and evaluation, pgs. 589-596.

LOURENÇO A. C., FIGUEIRAS F., DAS S., AMARAL J. S., KAKAZEI G. N., KARPINSKY D. V., SOARES N., PERES M., PEREIRA M. J., SANTOS N. M., TAVARES P. B., SOBOLEV N. A., AMARAL V. S., KHOLKIN A. L. (2010) Low Temperature Deposition of Ferromagnetic Ni-Mn-Ga Thin Films From Two Different Targets via RF Magnetron Sputtering, Mater. Res. Soc. Symp. Proc. Vol. 1250, G08-02.

Patents/propotypes

REGO R., OLIVEIRA C. - Catalisadores de ligas de paládio para cátodos de pilhas de combustível e respectivo método de produção. Patente de invenção nacional nº 105193; Ref. DMP/01/2010/264191. Deposit date: 06/12/2010.

REGO R., OLIVEIRA C. - Palladium alloy catalysts for fuel cell cathodes and a method of preparing the same. Pedido de Patente Internacional. Número de Pedido: PCT/IB2010/055605. Deposit date: 06/12/2010.

Organization of conferences

NAZARÉ PEREIRA A. M., TAVARES P. B., OLIVEIRA M. C., SILVA P. L., FERNANDES L., 5th Course of Electronic Microscopy in UTAD, Transmission Electron Microscopy (Materials Analysis in TEM), Vila Real, UTAD, 13 de Julho de 2010. Invited speaker: Paulo Ferreira, Univ. of Texas at Austin.

Internationalization

Collaborative publications/work with:

Departament de Química Física, Facultat de Química, Laboratori de Ciència i Tecnologia Electroquímica de Materials da Universitat de Barcelona (LEMMMA-UB), Barcelona, Spain (Prof. Dr. Pere Cabot);

Centro de Tecnologías Electroquímicas (CIDETEC-IK4) do Parque Tecnológico de San Sebastián, Spain (Dr. Francisco Alcaide);

Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, Czech Republic (Prof. Dr. Vladimír Matolin);

École de Chimie de Montpellier (Montpellier, France) (M. W. Chi Man, X. Cattoën)

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

Department of Applied Chemistry, Waseda University (Professor Kazayuki Kuroda), Tokyo, Japan

Institute of Physics, ASCR, Na Slovance 2, 18221 Prague 8, Czech Republic (V. Goian, S. Kamba, C. Kadlec, D. Nuzhnyy, P. Kuzel)

Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur 208016, India (Anil Kumar)

Laboratoire des Matériaux et du Génie Physique, MINATEC, Grenoble Institute of Technology, CNRS, 38016 Grenoble, France (J. Kreisel)

Swiss-Norwegian Beam Lines, European Synchrotron Radiation Facility (ESRF), 38000 Grenoble, France (D. Chernyshov)

Jozef Stefan Institute, Department of Nanostructured Materials, Jamova 39, SI-1000 Ljubljana, Slovenia (Goran Drazic)

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, PTDC/QUI/66012/2006. 94 743 €, (2009/11)

Thienylpyrroles as building blocks on the synthesis of organic and coordination compounds with NLO applications, PTDC/QUI/66251/2006. 8 000 €, (2009/11)

Surface Photochemistry, PTDC/QUI/65510/2006. 14066 € (2008/11)

Surface Photochemistry, PTDC/QUI/70153/2006. 11580 (2009/12)

Affinity Interactions between Cyanine Dyes and Biomolecules in Chromatographic Processes, FCT (2010/12), total: 54 624 €

A lipidomic approach of Alzheimer's disease - Study of lipid profile changes in brain mitochondria. PTDC/SAU/115865/2009. (2011/13). 96 326 €.

Study of structural modifications induced by thermal and oxidative degradation in oligo and polysaccharides by advanced mass spectrometry: (FCT 2010/13) 33 612 €.

Quality Study of the national beeswax. Adulteration detection by FTIR and GC-MS (2009/10). 47 980 €

Protein Concentrates for Aquaculture - Projecto Eureka – EUProteinAQUA. QREN (2010/12). 130 000 €.

NutriDouro. Confitage techniques of fruits and vegetables without sucrose or with a reduced content of sucrose, and impregnation of healthy constituents. QREN (UTAD/DouroMel). (2010/13) 565 751 €

Objectives & Achievements

Objectives

1. Synthesis and structural characterization of organic compounds with applications in photochromic devices and pharmaceuticals.
2. Synthesis and structural characterization of new 2H-chromenes with fused aromatic rings and benzo[1,3]oxazines
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 , ^{13}C and ^{19}F -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 sp^3 carbon.
8. Synthesis of new functional dyes (mainly of the squarylium and croconylium type) as sensitizers for Photodynamic Therapy, as fluorescent near-infrared probes for biomolecules and as pseudo-affinity ligands for Affinity Chromatography.
9. The research objectives of the Food Chemistry are a multidisciplinary approach to food quality, functional properties and health benefits. Taking into account new challenges in the relationship between food and health, our research goals are the study of the chemical composition of foods, chemical changes during processing and relation to their functional properties, namely, coffee (melanoidins) mushrooms (anticancer polysaccharides) apples, olives and chestnuts (ascorbic acid and polyphenolic compounds antioxidant activity). In this line also new healthy food formulations (candy fruits) and the use of agricultural byproducts to the development of nutraceuticals (mushroom dietary fiber) are other important goals of the group.
10. 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).
11. Study of lipid profile changes in brain mitochondria isolated from mouse 3xTg-AD, a model to Alzheimer's Disease.
12. Farmacological and kinetic evaluation of tacrine derivatives. Study of lipid profile changes in brain (cortex) of rats treated with tacrine and two new compounds derived from tacrine.
13. Study of cardiolipin alterations by electrospray tandem mass spectrometry of kidney mitochondria isolated from Wistar rats treated with gentamicin, a nephrotoxic drug.
- 14 - Assessment of the impact of production technology on the chemical composition of fermented beverages.

Main Achievements

Hydrophilic interaction chromatography using a TSKgel Amide-80 stationary phase with isocratic elution was successful in resolving ascorbic acid (AA) and the epimeric isoascorbic acid (IAA). This simple, fast, and robust hydrophilic interaction chromatography-DAD method was applied for the analysis of several food products. The method was fast, accurate, and precise with a LOQ(AA) of 1.5 mg/L and LOQ(IAA) of 3.7 mg/L.

The effects of industrial processing on the composition of minerals, free sugars, vitamins and pigments in fruits of chestnut cultivars were evaluated. Fruits from both harvest years had a significant content of free sugars, with sucrose predominating, and these sugars were more affected by the processing stage. Significant levels of lutein, lutein esters, gamma-tocopherol and vitamin C were also found in the chestnut

fruits. Fruit carotenoids and vitamin C significantly decreased during the industrial processing.

The galactomannans purified from coffee infusions have been shown to present in vitro immunostimulatory activity on murine B- and T-lymphocytes. These properties have also been shown characteristic of the galactomannans recovered from coffee residue by strong alkali solutions and rendered soluble in water by partial acetylation. It was found that the galactomannans have a comparable molecular weight (90-110 kDa), and similar glycosidic-linkage composition.

A series of new substituted benzo[1,3]oxazines presenting bulky substituents were prepared. Laser irradiation of these uncoloured compounds in solution promotes the cleavage of the C-O bond and the opening of the [1,3]oxazine ring generating a zwitterionic species that absorbs strongly at 440 nm. The photogenerated coloured open isomers are thermally unstable and revert to the initial closed form with first order kinetics and lifetimes ranging from 13 to 68 ns.

Two new unexpected photochromic compounds were obtained from naphtho[2,1-b]pyran-1-one 1. UV irradiation of the new compounds provided thermally stable photoproducts that returned to the initial uncoloured forms under visible irradiation. The photochromic behaviour of these compounds and the structures of the photoproducts formed in these reactions were characterized by 1D and 2D NMR.

A new naphtho[1,2-b]pyran possessing an ester substituent in position 4 was prepared and then converted to the carboxylic acid derivative. The photochromic behaviour of these two compounds was studied by UV-vis spectroscopy and the structures of the photoproducts elucidated by NMR. In strong acid medium both compounds were converted to a spiro derivative formed through the opening of the pyran ring followed by an intramolecular lactone ring formation and electrophilic aromatic substitution.

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. We have found differences in the fragmentation mechanism of carbazole, dibenzofuran and dibenzothiophene derivatives with the same annelation. Our results suggest the involvement of the allenyl-naphthol intermediate on the photochromic mechanism.

The crystal structure of a squarylium cyanine dye derived from benzoselenazole and the crystal structures of squarylium dyes substituted at the central four-member ring were determined for the first time by X-ray crystallography.

Several aza-substituted squarylium dyes were studied as 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). Aza-substituted squaraines for the fluorescent

Sixteen yeast-derived aroma compounds contributing to the sensorial quality of mead were identified and quantified. Global analysis of aromatic profiles revealed that the total concentration of aroma compounds in meads was higher in those fermentations where diammonium phosphate was added. A positive correlation between nitrogen availability and the levels of ethyl and acetate esters was observed.

The effect of the refermentation process (mixture of acidic wine with musts from freshly crushed grapes or with residual marc) and micro-oxygenation on the efficiency of acetic acid removal and on wine aroma composition was studied. The aroma compounds content of deacidified red wines was dependent on the refermentation process employed rather than on micro-oxygenation.

Group Productivity

Publications in peer review Journals

- BARROS, A.I.R.N.A., Silva, A. P., GONÇALVES, B., NUNES, F. M. (2010) - Fast, Simple and Reliable Hydrophilic Interaction Liquid Chromatography Method for determination of Ascorbic and Isoascorbic Acids, *Analytical & Bioanalytical Chemistry* 396, 1618-2642.
- COELHO P.J., FERNANDES I.C, CARVALHO L.M. (2010) - Synthesis of Carbonyl Dyes from 1-Hydroxy-2-acetonaphthone and 2-Fluorobenzophenone. *Journal of Heterocyclic Chemistry* 47, 1123-1126.
- COELHO P.J., CARVALHO L.M., GONÇALVES L.F., SILVA C.R., CAMPOS A.M., GOMES M.J. (2010) - Photochromic hybrid sol-gel films containing naphthopyrans. *Journal of Sol-Gel Science & Technology* 56, 203-211. (IF 2009 = 1.393)
- FERREIRA LMM, CELAYA R, SANTOS AS, FALCO V ET AL. (2010) - Comparison of long-chain fatty acids and alkanes as markers to estimate diet composition of equines and cattle consuming heathland vegetation species. *Livestock Science*, 131, 2-3, 260-271
- FERREIRA LMM, CELAYA R, FALCO V, ET AL. (2010) - Evaluation of very long-chain fatty acids and n-alkane epicuticular compounds as markers for estimating diet composition of sheep fed heathland vegetation species. *Animal Feed Science and Technology* 156, 3-4, 75-88.
- MENDES-FERREIRA A; COSME F; BARBOSA C; FALCO V; INES A; MENDES-FAIA A; (2010) Optimization of honey-must preparation and alcoholic fermentation by *Saccharomyces cerevisiae* for mead production. *International journal of food microbiology* 144, 1, 193-198
- NUNES F. M., COIMBRA M.A. (2010) - Role of hydroxycinnamates in coffee melanoidin formation, *Phytochemistry Reviews* 9, 171-185.
- OLIVEIRA M. M., CARVALHO L. H.M., PEIXOTO F., OLIVEIRA-CAMPOS A., REIS A., DOMINGUES P., DOMINGUES M. R. M. (2010) - Cleavages of photochromic compounds derived from heterocycles under Electrospray Tandem Mass Spectrometry: Study of the influence of the heteroatom in fragmentation mechanisms, *Rapid Communications in Mass Spectrometry* 24, 2171-2174.
- PROSTOTA Y., COELHO P.J., PINA J., SEIXAS DE MELO J. (2010) - Fast photochromic sterically hindered benzo[1,3]oxazines. *Journal of Photochemistry and Photobiology A: Chemistry* 216, 59-65.
- SALAHELDIN A. M., OLIVEIRA-CAMPOS ANA M. F., RODRIGUES L. M., OLIVEIRA M. M., PEIXOTO F. P. (2010) - Synthesis of New Tacrine Analogues from 4-Amino-1H-pyrrole-3-carbonitrile, *Helvetica Chimica Acta* 94, 242-248.
- SIMÕES, J.; NUNES, F.M.; DOMINGUES, M.R.; COIMBRA, M.A. (2010). Structural features of partially acetylated coffee galactomannans presenting immunostimulatory activity, *Carbohydrate Polymers* 79, 397-402.
- SOUSA CM, COELHO PJ, CARVALHO LM, VERMEERSCH, G., BERTHET, J., DELBAERE, S. (2010) - Unexpected formation of new photochromic compounds derived from 3,3-diphenyl-3H-naphtho[2,1-b]pyran-1-one, *Tetrahedron* 66(42), 8317-8324.
- SOUSA C.M., COELHO P.J., VERMEERSCH G., BERTHET J., DELBAERE S. (2010) - Synthesis and photochemical reactivity of new 4-substituted naphtho[1,2-b]pyran derivatives. *Journal of Photochemistry and Photobiology A: Chemistry* 216, 73-78.
- DE VASCONCELOS M. C. B. M., NUNES F., VIGUERA C. G., BENNETT R. N., ROSA E. A. S., FERREIRA-CARDOSO, J. V. (2010) - Industrial processing effects on chestnut fruits (*Castanea sativa* Mill.) 3. Minerals, free sugars, carotenoids and antioxidant vitamins, *International Journal of Food Science & Technology* 45, 496-505.
- VILELA-MOURA A, SCHULLER D, FALCO V, ET AL.(2010)- Effect of refermentation conditions and micro-oxygenation on the reduction of volatile acidity by commercial *S. cerevisiae* strains and their impact on the aromatic profile of wines. *International Journal of Food Microbiology* 141, 3, 165-172

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:

BARROS, Ana, NUNES, Fernando, FRAGA, Sara. Method for production of mushroom dietary fiber from mushroom wastes and left overs, with sensorial and functional properties to be used as a food ingredient. International Patent PCT/IB2009/055552, 07-12-2009.

Organization of conferences

Dia Mundial da Alimentação. Organização Núcleo de Estudantes de Ciência Alimentar e Coordenação da Licenciatura em Ciência Alimentar. UTAD, Vila Real, 18 de Outubro de 2010. Ana Barros

III Jornadas de Bioquímica da UTAD, 21-22/4/2010, M.M Oliveira (CQVR)

Projecto Ciência Viva - Ocupação Científica dos Jovens nas Férias (OCJF), Maria João Melo de Carvalho:

•Projecto nº 2126 – Doença de Alzheimer, na descoberta da cura. Investigadores responsáveis – Maria Manuel Oliveira e Romeu António Videira
Financiamento (Ciência Viva)– 1000 €

•Projecto nº 2196 – Síntese e Purificação de um corante com potencial tratamento do cancro. Investigador responsável – Lucinda Vaz dos Reis.
Financiamento (Ciência Viva) – 1000 €

Industry contract research

Protein Concentrates for Aquaculture - Projecto Eureka – EUProteinAQUA. QREN (2010-2012). 130 000 €.

NutriDouro (Técnicas de confitagem de frutos e vegetais sem sacarose, ou com um conteúdo reduzido de sacarose, e impregnação de constituintes saudáveis). QREN (UTAD/DouroMel). (2010-2013) 565 751 €.

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;

Daniel Lynch (Exilica Limited, UK).

Algirdas Sackus, Kaunas University of technology, Lithuania

Michel Frigoli. Université de Versailles.

Stefan Pierzynowski. Institute of Agricultural Medicine Lublin, Poland.

Government/Organization contract research

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

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

Viticulture sustainability in Douro/Duero region. INTERREG €411 433 (2009/11)

BioCombus – Recovery of Wastes as Bio Fuel, Project nº 3483, (QREN) 1 168 574 € (2008/11).

Development of new fertilizers to agriculture, CUF, Adubos de Portugal. 10 000 € (2010)

Modelling nitrogen mineralization in Eucalyptus globulus stands, RAIZ, Instituto de Investigação da Floresta e do Papel. 10 000 € (2010)

The bioavailability of P in soils derived from volcanic rocks. Secretaria Regional da Agricultura e Pescas dos Açores. €4000.

EcoCidadania – Ecological Citizenship (ONG- Componente ambiente) 2008/10 €9600.

SeivaCorgo – Intervention Project on the River Basin Corgo. ON.2 Programme (2007/13) €98 120

Effect of phytochemicals on the organic residues transformation and on key processes of the C and N cycles. PTDC/AGR/102006/2008. €125 680. (2010/12)

Gaseous emissions measured in irrigated rice fields produced in two different soils in Portugal: the effect of cultural practices, climate and the increased concentration of CO₂ in the atmosphere. FCT: PTDC/AGR/102529/2008. €45 360. (2010/12)

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, pulp and paper mill 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. Adsorption of heavy metals in low cost biosorbents (algae *Sargassum muticum*). Compare the effectiveness of adsorbent prepared for removal endocrine disruptors compounds and pesticides from water.

3. To perform comparative studies of the removal of endocrine disruptor compounds (17 β -estradiol and Bisphenol A) from water using agroforestry wastes.
 4. Study the sorption kinetics of Polycyclic Aromatic Hydrocarbons (PAHs) over plants tissues (biomarkers).
 5. To study the influence of time scale on geochemical processes.
 6. 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.
 7. Research on treatment, recovery and valorisation of industrial by-products and wastes under an industrial ecology approach.
 8. 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 O₃, O₃/UV and O₃/UV/H₂O₂ in a pilot-scale bubble column reactor; (2) combining long term aerated storage (biological process) and coagulation/flocculation. Were also studied the decolouration of orange II solutions by TiO₂ and ZnO active layers screen-printed on ceramic tiles under UV radiation. A brief review related to the decolorization of textile azo dyes by yeasts was performed and published as chapter book. Finally, we developed a photochemical degradation study of three commercial azo dyes used in the textile industry.
2. Sorbents prepared from pine bark and almond shell proved to be effective for the removal of 17 β -estradiol and Bisphenol A from aqueous solutions. Particle size and pretreatment were found to be of considerable significance. The experimental results show that pine bark and almond shell powders pretreated with formaldehyde present higher adsorption efficiency, followed by pine bark and almond shell washed with hot water.
3. Despite Gas Chromatography coupled with Mass Spectrometry (GC-MS) is the prevalent method for the analysis of PAHs, two different environmental sampling strategies have been used (direct sampling of the air and biomarkers). Generally, the measurement of PAHs foliar uptake is compared to the amount determined by GC-MS from samples of surrounding air. However, very few kinetics studies have been conducted, in part because of the challenges associated with the delivery of these pollutants. In 2010 different PAHs vapor generators setup were tested, and a new system were developed.
4. Optimization of the BioCombus technology. In a previous research we use only olive mill and cork wastes and several new formulations and its relevance in the calorific value were now tested using other wastes or by-products. We analyse the potential inclusion of olive lives from olive oil industry, grape husks and grape seeds from winery industry, chestnut shell (outer shell and inner skin) from chestnut industry.
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.
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

BRAZ, R.; PIRRA, A.; LUCAS, M.S.; PERES, J.A.; (2010) - Combination of long term aerated storage and chemical coagulation/flocculation to winery wastewater treatment, *Desalination* 263, 226-232. (IF 2009 = 2.304)

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CLARO J. (2010) - Processo e instalação para a produção industrial de blocos, pastilhas e granulados a partir de resíduos de origem vegetal. Pedido Patente Nacional PT 105275 (Patente pendente). Titular do pedido de patente: UTAD.

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10th National Meeting on Photochemistry, Universidade do Porto, Porto, 9-10 December 2010. Member of Organizing 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, QREN N° 3483, PI: J.C. Claro. 1 168 574 €. (10/2008 - 09/2011).

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

Internationalization

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.