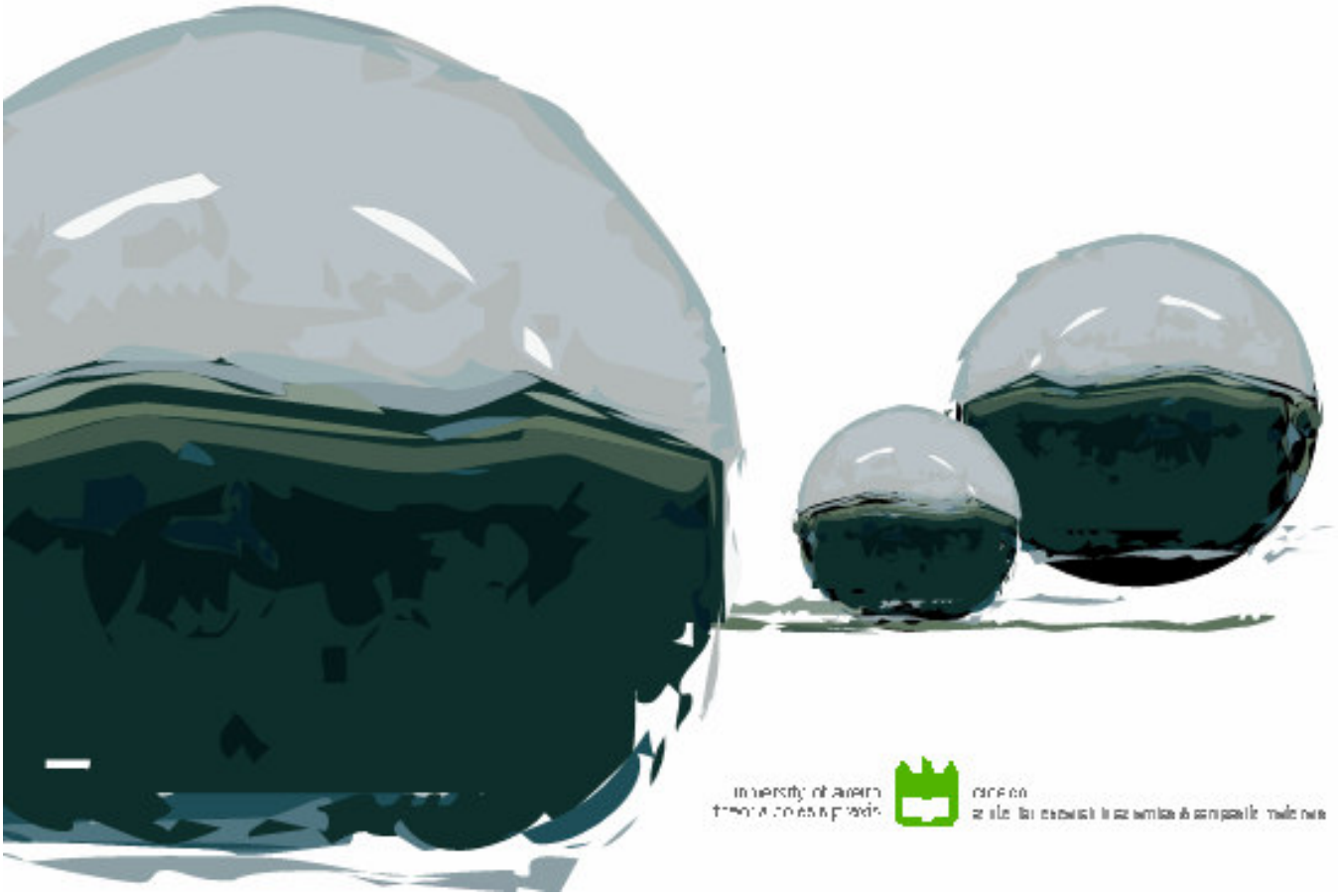
Activity Report '07
Activity Plan '08

Centre for Research in Ceramics and Composite Materials
Associated Laboratory

CICECO



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INTRODUCTION

The associate laboratory CENTRE FOR RESEARCH IN CERAMICS AND COMPOSITE MATERIALS (CICECO) was created in 2000, in the University of Aveiro, Portugal, and received the status of Associated Laboratory of the Portuguese Ministry of Science, Technology and High Education on March 2002, with the mission of:

developing the scientific and technological knowledge necessary for the innovative production and transformation of ceramics and composite materials

Our main areas of expertise are:

Area 1: advanced micro- and nano-structured materials for communications technologies;

Area 2: advanced materials for industrial applications;

Area 3: biorefineries and biomaterials.

CICECO is one of the main Portuguese institutes in the field of materials science and engineering, in terms of the size of the Research Team and Scientific Output.

This document reports the main activities developed in 2007 and the actions aimed for 2008. A detailed list of publications, theses, projects and activities is provided in sections 4 and 5.

FACTS & NUMBERS

CICECO is one of the largest Portuguese institutes comprising on 31st December 2007, 284 people, which represents an increase of 6% over 2006 and 62% relatively to 2002 (Table 1); Almost 50% of the Research Team hold a PhD degree.

Table 1: CICECO's Research Team, 2002-2007

Research Team	2002	2003	2004	2005	2006	2007
Professors and Lectures	47	47	50	52	53	51
Full-Time Researchers	5	9	12	16	20	23
Pos-Doctoral Associates	23	22	29	47	46	46
PhD Students	54	60	61	51	67	69
MSc and Other Students	26	44	54	63	49	39
Laboratory Technicians	4	8	5	5	5	4
Administrative Personel	1	3	5	6	7	6
Collaboradors	16	13	12	10	23	46
TOTAL	176	206	228	250	270	284

Since 2002, 10 of our researchers were awarded the *'Prize for Scientific Excellence'* by the Portuguese Science Foundation, and two of the youngest CICECO researchers, received the prestigious prize *'Programa Gulbenkian de Estímulo a Investigação 2006'*, *'Prémio Celestino da Costa/ Jean'* and one of our professors became member of *'The Lisbon Academy of Science'*.

CICECO is also one of the most productive research institutes in the country in all scientific areas, with an average **PUBLICATION** of 4.5-5 SCI papers per year per academic staff or full-time researcher:

**** Over 1700 SCI papers published since 2002 (many in top journals);***

**** 304 SCI papers published in 2007;***

**** 36 patents published;***

**** 87 PhD theses terminated in the last 6 years (2002-07).***

Table 2 is a brief overview of the scientific activity outcome.

Sientific Activity	2002	2003	2004	2005	2006	2007	TOTAL
PhD Theses:	14	13	11	14	19	16	**87**
MSc Theses:	10	8	7	17	16	47	**105**
SCI Papers, IF >=5:	1	3	4	5	7	17	**37**
SCI Papers, IF<5:	204	225	283	310	376	287	**1685**
Books:	-	-	1	1	1	-	**3**
Books Chapters:	4	14	12	10	5	17	**62**
National Patents:	7	3	1	6	6	6	**29**
International Patents:	2	-	-	0	1	4	**7**

Table 2: CICECO's Scientific Output, 2002-2007

The number of **PROJECTS** in progress in 2007 was 77, similar to the last five years. The main sources of funding are FCT, *National Science Foundation* (75%), and the European Funding Agencies and Programmes, *European Commission, FEDER*, (14%). Section 5 lists all projects funded.

CICECO is a truly international research centre:

**** 48% of full-time researchers and 60% of Post-docs are not Portuguese;***

**** is part of the main stream materials research in Europe;***

**** participates in Networks of Excellence, such as FAME - 'Functionalised Advanced materials and Engineering of Hybrids and Ceramics';***

**** runs two Erasmus Mundus MSc courses;***

**** harboured one of the first Portuguese Marie Curie Trainning sites.***

CICECO is also commited to knowledge transfer to industry through our Centre for Materials Design and Technology.

CICECO is probably the best equipped institute in the country to perform research in materials science. In particular, we are the focal point of the Portuguese Electron Microscopy Network and also house the top solid-state nuclear magnetic resonance facilities. We are also one of the best equipped national centres for X-ray diffraction.

In 2007 several activities were performed by CDTM, in order to promote technology transfer from CICECO and, thus, contribute to the national economic development. The cooperation with industry, by means of R&D contracts and/or technical services, enabled the development of strong links with companies. 14 new industrial contracts were established, representing a net income of about 320 k€, a considerable increase relatively to 2006 (ca. 140k€). Several programmes of cooperation were also established with companies, enabling future research projects.

Strengthening the long lasting cooperation with companies was incremented through the technology platform **IDPoR – Research and Development in Polymers from Renewable Resources**. Formalised in September 2006, IDPoR has developed during 2007 several activities aimed at fulfilling its objectives and strengthening its structure.

In the Ceramics area, CDTM has been promoting the constitution of a **Competitive Ceramic Pole**, in close cooperation with the French Competitiveness Pole of Ceramics, in Limoges. We anticipate that in 2008 the formation of this pole will be completed or much advanced.

The activities for the implementation and management of the **National Electron Microscopy Network (RNME)** were also of major importance for the visibility of CICECO amongst other R&D centres and society overall. The first training initiatives of this network, coordinated by Prof. Dr. Joaquim M. Vieira and managed by CDTM staff, had high attendance and future activities are being planned.

The protection of CICECO´s technologies through patenting was, high in in our priorities. In this respect, CDTM provided consultancy and technical expertise to CICECO researchers. In 2007, CICECO filled 9 patent applications, representing an increase of 50%, comparing with 2006 (6 patents), concerning the protection of new-to-the-World products and processes.

CDTM assisted the establishment and growth of the spin-off **FoodMetri**c in the management area. In its first year of activity, this company gave the first steps towards addressing its market by presenting new products. Besides FoodMetric, CDTM has also been involved in the creation of two new spin-off companies, based on technologies developed by CICECO´s researchers.

Regarding the participation of CICECO in the EC framework Financing Programme (2007-2013), CDTM was much involved in screening and scanning the best programmes for CICECO researchers and in promoting their participation by giving support in several stages of the development of project proposals. In the case of the 7th Framework programme, CDTM staff provided support to 20 new proposals, in different calls. At national level, CDTM was involved in the development of 3 proposals to the new programme QREN ("Sistemas de Incentivos às Empresas" calls) and one to the regional operational programme for the Centro Region iCentro. Concerning the search of opportunities to support technology transfer at CICECO, CDTM produced three project proposals to different instruments: Capacity Programme of 7FP, Pilot projects for cooperation between European Institutes of Technology and Interreg programme.
Also important in year 2007 was the promotion of CICECO in the society, a crucial fact for the recognition of CICECO as one of the most important Materials R&D centres in Portugal. The participation of CDTM in two national events aiming at the promotion of research and in 20 national/international events was of great importance for our recognition outdoors. Also vital for this purpose was the organization of technical workshops and seminars, an important element of connection of academy to industry and society in general. The CDTM has organised 15 seminars in the ceramics and composite materials areas.

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SECTION 2
Activity Report 2007

Area 1 - Advanced Micro- and Nanostructured Materials for Communications technology
Area 2 - Advanced Materials for Industrial Applications
Area 3 - Biorefineries and Biomaterials

INORGANIC FUNCTIONAL NANOMATERIALS AND ORGANIC-INORGANIC HYBRIDS

New Microporous Materials. ETS-10 and AM-2 powders and membranes have been prepared from clear solution. Membranes have been prepared on porous alumina tubular supports. Well intergrown ETS-10 and AM-2 membranes with a thickness of *ca.* 2.5 μm have been obtained after 24 and 15.5 h, respectively. Y and Eu have been successfully incorporated into microporous zirconosilicate with petarasite structure. This structure type is suitable for Ln ions incorporation, therefore is a suitable system for the preparation of new multifunctional luminescent materials.

The Hg^{2+} uptake from water of microporous and layered titanosilicates has been studied and found to be ETS-4 > ETS-10 > AM-2 and AM-4. The kinetics of the Hg^{2+} removal follows a pseudo second-order model. Ca, Na and Mg ions do not reduce the Hg^{2+} uptake capacity of ETS-4 while high Cl^- concentrations greatly decrease the Hg^{2+} sorption capacity of ETS-4.

The structure of the layered, non-centrosymmetric titanosilicate AM-1, $Na_4Ti_2Si_8O_{22}{\cdot}4H_2O$, has been refined from single-crystal XRD data. The hydrogen atom has been located for the first time.

The M-doped (M = Y and Eu) microporous zirconosilicate AV-3 materials, possessing the structure of mineral petarasite and with Zr/M ratio of 4, have been prepared via hydrothermal synthesis. The structure of these materials contains elliptical channels, running down the b- and c-axes, defined by mixed six membered rings, consisting of pairs of SiO_4 tetrahedra linked by ZrO_6 octahedra. There are also six-membered silicate ring channels running parallel to the c-axis. M ions predominantly occupy Zr positions, sitting on the channel surface and making AV-3 a proper system to create new multifunctional photoluminescent materials.

Upon dehydratation, the layered lanthanide silicates $K_3[LnSi_3O_8(OH)_2]$, Ln) Y, Eu, Tb, and Er, tranform into small-pore framework $K_3LnSi_3O_9$, Ln) Y, Eu, Tb, and Er solids, named AV-23. The photoluminescence, radiance, and lifetime values of AV-23 have been studied and compared with those of AV-22. Both materials have a similar chemical makeup and structures sharing analogous building blocks, hence providing a unique opportunity for rationalizing the evolution of the PL properties of lanthanide silicates across dimensionality.

The European Commission has issued directives restricting emissions of chlorinated compounds associated to the production of PVC. Normally, EC is present in low levels in the effluent from the synthesis of PVC becoming an impurity preventing the recycle of this current to the reactor. The required purification step is not easy to achieve through conventional processes. We have been investigating adsorption routes for the purification of VC by adsorbing EC on a crystalline microporous adsorbent known as aluminum methylphosphonate polymorph alpha (AlMePO-α). The individual adsorption isotherms of VC and EC were measured and Grand Canonical Monte Carlo simulations were performed. The results support the use of the AlMePO-α as an appropriate adsorbent for the purification process of VC, upholding the selective adsorption of EC.

Layered Materials. A new template-free layered Mn(III) phosphate, $Na_3MnH(P_{0.9}O_4)_2$, has been synthesized. The crystal structure was solved *ab initio* from powder XRD data. This material is paramagnetic above 50 K.

The synthesis and the characterization of layered materials (LHD´S), as well as the intercalation of metal and metallorganic compounds into LDHs) has been accomplished. The photofunctional and/or catalytic properties of several of these materials have continued to be studied.

Nanostructured Materials. We have investigated the relationship between nanostructure and optical properties on epitaxial thin films and low-dimensional heterostructures of wide bandgap semiconductors with technological interest for light emission. Device structures, which include single- and multiple-quantum wells, were studied by high-resolution X-ray diffraction in order to gain an insight regarding the effects of strain and composition on various material physical properties relevant in terms of device performance and functionality. Moreover, we have used the nitride light emitting backplanes, as a platform to integrate other material systems, namely metallic nanocrystals, achieving nanostructures tailored with nanometre scale control. We have also performed theoretical calculations to predict the size effect on the melting temperature of nanomaterials, namely for the case of ZnO nanostructures.

A combination of SEM and (HRTEM was used for the characterization of advanced materials, ranging from organic materials to organic-inorganic hybrid materials, thin films and diluted magnetic semiconductor (DMS) nanoparticles. In addition to standard imaging and diffraction techniques also spectroscopic and spectrometric techniques such as EDS and EELS were applied. By a combination of these techniques the distribution of the dopant atoms in the zirconia and zinc oxide host structures were analyzed at high spatial resolution.

The work on rare-earth ordered nanocrystalline hybrid structures was continued especially by intercalating new organic moieties, performing advanced structural and optical characterization techniques. By changing the intercalated species we could modify the optical properties of these materials. Furthermore, other kind of luminescent hybrids and inorganic nanoparticles was synthesized by similar methods. For example, lanthanide doped strontium and barium aluminates were recently synthesized.

Synthetic studies of gold nanoparticles attached onto wood or bacterial cellulosic fibres have been performed in situ in the presence of the fibres or by polyelectrolyte-assisted deposition. The optical properties of the final nanocomposites could be tailored not only by the starting Au nanoparticles characteristics but also by the preparative method associated to the type of cellulosic fibres used as the substrate. Thus, gold nanoparticles assembled or generated in situ within cellulosic fibres, are excellent components for long term optical and chemically stable nanocomposites, which appear particularly interesting for security paper applications.

Magnetic latexes were prepared by the encapsulation of organically capped $CoPt_3$ nanoparticles via miniemulsion *in situ* radical polymerization of *tert*-butyl acrylate (*t*BA). This is the first example of a $CoPt_3$ based polymer nanocomposite showing ferromagnetic behavior at room temperature. Each nanocomposite particle contains a magnetic core composed of $CoPt_3$ nanoparticles (d ~ 7 nm, a_0=3.848 Å) encapsulated by poly(*t*-butyl acrylate). The $CoPt_3$/P*t*BA latexes contain polyester groups that can be readily hydrolyzed, rendering the surface with carboxylic functionalities and hence allowing bioconjugation. Complementary to such surface modification experiments, we report that bovine IgG antibodies can bind to the magnetic latexes and the potential of the nanocomposites for *in vitro* specific bioapplications is discussed.

Non-Aqueous Chemistry Applied to Atomic Layer Deposition. A new non-aqueous sol-gel approach applied to the atomic layer deposition technique was developed in order to synthesize various metal oxide materials on different substrates. Such a novel approach brought several advantages compared to ordinary deposition techniques namely a very low deposition temperature, the ability to avoid a SiO_2 interfacial layer during the growth of an oxide on a silicon substrate and the possibility to precisely control the film thickness.

Polyoxometalates. New hybrid compounds with polyoxometalates(POMs) and organic moieties: compounds were prepared and characterized with the heteropolyanions $[XM_{12}O_{40}]^{n-}$ (M = Mo, W, X = P, Si) and caffeine or

$[PW_{11}O_{39}]^{(n+6)-}$ and 1-butyl-3-methylimidazolinium. Preparation of supported iron polyoxotungstates: the anions were supported in silica by two different procedures. Studies on the homogeneous catalytic oxidation of hydrocarbons with H_2O_2: catalytic oxidation of alkylbenzenes (*p*-cymene, cumene and sec-butylbenzene) and alkylnaphtalenes (1-ethylnaphtalene, 2-ethylnaphtalene) were performed with iron polyoxotungstates like $[XW_{11}Fe(H_2O)O_{39}]^{n-}$, X = P, Si and B, and others.
Following our research interest in materials containing lanthanide cations and Keggin-type POMs, we have been studying the preparation of new organic-inorganic hybrid coordination compounds containing lanthanides, POMs and an organic ligand. One of our aims is to investigate the types of crystalline networks that can possibly be obtained. We have prepared a series of organic-inorganic hybrid materials composed by α_2-lacunary Wells-Dawson polyoxotungstate lanthanide complexes and 3-hydroxypicolinic acid. In this type of hybrid materials, the lanthanide luminescence may be sensitized by both the 3-hydroxypicolinate ligand and the polyoxometalate moiety.

Novel Luminescent Systems. New lanthanide(III) complexes (Ln= Sm, Tb and Eu) of picolinic acid and glutaric acid were prepared and characterised. The crystal structure of the complex $[Sm(glu)(pic)(H_2O)_2]$ (where Hpic and H_2glu stand for picolinic and glutaric acids, respectively) was determined by single-crystal X-ray diffraction studies. All the Ln complexes were characterised by elemental analysis, infrared spectroscopy, X-ray powder diffraction and thermoanalytical measurements, and together the data show that these Ln complexes are isostructural. The effect of both organic ligands on the photoluminescence behaviour of the Sm^{3+}, Eu^{3+} and Tb^{3+} complexes is discussed and we anticipate the possibility to vary the photoluminescence of picolinic-containing lanthanide compounds in which the length of a also present bridging ligand could be systematically varied.

Crystal Engineering of Organic-Inorganic Hybrid Materials. Lanthanide diphosphonates, $[H_3N(CH_2)_4NH_3]Ln[hedpH][hedpH_2]$ (Ln = La, Eu, Tb; hedp = 1-hydroxyethylidenediphosphonate), have been synthesized and their structure characterised.The crystal structure consists of polymeric La[hedpH][hedpH2] single chains built up from vertex-sharing LaO_7 polyhedra and CPO_3-tetrahedra. The chains are cross-linked by strong hydrogen bonds to form a three-dimensional network with large channels containing the template cations. The photoluminescence properties of the Eu and Tb materials have been studied.
The following metal-organic frameworks containing lanthanide centres have been prepared via mild hydrothermal synthetic approaches and characterised in the solid-state using X-ray diffraction (single-crystal and powder), vibrational spectroscopy (FT-IR and FT-Raman), thermoanalytical studies, electron microscopy (SEM and EDS), and CHN elemental composition: $[Ln(H_3NMP)]\cdot 1.5(H_2O)$ (2D network) [Ln = La, Pr, Nd, Sm or Eu; H_3NMP^{3-} is a residue of nitrilotris(methylenephosphonic acid)]; $[Ln(glu)(pic)(H_2O)_2]$ (1D polymer) (Ln = Sm, Tb and Eu; Hpic and H_2glu stand for picolinic and glutaric acids, respectively). In the case of the former family of materials, the structural details could only be unveiled from the combination of high-resolution powder XRD data (from a synchrotron source) with solid-state NMR data. The photoluminescence properties of these two families of materials were studied at ambient and low temperature.
The first examples of complex-based heterodimetallic crystalline compounds containing $[Ge(C_2O_4)_3]^{2-}$, $[M(phen)_3][Ge(C_2O_4)_3]\cdot xH_2O$ (where M = Cu, Fe, Ni, Co; phen is 1,10'-phenanthroline), and binuclear complexes containing the neutral $[Ge(C_2O_4)_2]$ moiety connected by two μ_2-OH groups to a $[M(phen)_2]^{2+}$ fragment, $[MGe(phen)_2(\mu_2\text{-}OH)_2(C_2O_4)_2]$ (where M = Cd and Cu), have also been reported.

A combination of physical methods were used to characterise the organotin compounds $[((Me)_2(menthyl)Sn)_2MoO_4(H_2O)_{3.5}]$ and $[Me_3SnVO_3]$. EXAFS studies revealed that the organotin molybdate is polymeric and contains $[MoO_4]^{2-}$ tetrahedra coordinated to $[R_3Sn]^+$ cationic spacers. ^{51}V and ^{119}Sn MAS NMR spectra for the organotin vanadate were in agreement with the structure determined by a full Rietveld refinement using conventional powder XRD data. Both compounds function as selective and recyclable solid catalysts for the liquid-phase epoxidation of olefins by *tert*-butylhydroperoxide.

Organic-Inorganic Hybrids Lacking Activating Centers. Hierarchically organized bilayer mono-amidosil consisted of 2D siliceous domains, separated by perpendicularly oriented alkyl chains, self-assembled through (i) intermolecular hydrogen bonding; (ii) partially interdigitated van der Waals packing, and (iii) an entropic term related to the phase separation. This hybrid exhibited a reversible order–disorder phase transition achieved by heating/cooling cycles between room temperature and 120 °C, which induced hysteretic behavior of the emission energy, following a logarithmic time dependence. The emission energy's logarithmic time dependence reflected hierarchically constrained dynamics without any characteristic microscopic time, supporting therefore the nanoscopic sensitivity of the monoamidosil photoluminescence.
The energy transfer mechanisms that occur in the white-light emission of sol-gel derived amine- and amide-functionalized hybrids were quantitatively addressed. The white-light photoluminescence results from a convolution of the emission originated in the NH/C=O groups of the organic/inorganic cross-links with electron-hole recombinations occurring in the siloxane nanoclusters, both emissions typical of donor/acceptor pairs. The energy transfer rate was quantitatively estimated for d-U(600) (the di-ureasil host with smaller number, 8.5, of polymer repeat units) generalizing the ideas proposed recently for the intramolecular energy transfer between singlet and triplet ligand levels and ligand-to-metal charge transfer states in lanthanide coordination compounds. The dipole-dipole energy transfer rate between the two emitting centers is 1.3×10^9 s^{-1}, larger than the value estimated for the transfer rate mediated by the exchange mechanism, 3.7×10^8 s^{-1}. The predicted room-temperature emission quantum yield of that di-ureasil hybrid is comparable to the corresponding experimental value (7 ±1 %), pointing out a strong dependence of the radiative component values of the two emissions with temperature, induced by the glass-rubber phase transition of the hybrid's polymer chains. To the best of our knowledge, this is the first attempt to explicitly quantify the energy transfer rate between distinct hybrid emitting centers. The detailed characterization of these energy transfer mechanisms will definitively contribute to the recognition of the paths needed for the development of siloxane based hybrids characterized by interesting photonic features and high-light emission efficiency. Moreover, the procedure reported provides a theoretical scheme that might be useful in guiding the interpretation of experimental data and in the modeling of new organic-inorganic hybrids.

New Hybrid Materials. Sol-gel derived highly photostable luminescent poly(ε-caprolactone)siloxane biohybrids (PCL(530)/siloxane)) doped with $Eu(tta)_3(H_2O)_2$ (where tta- is 2-thenoyltrifluoracetonate) and $Eu(tta)_3$phen (where phen is 1,10-phenantroline) complexes, and in situ synthesis of Euphen complex in urea cross-linked organic/inorganic di-ureasil hybrids via carboxylic acid solvolysis were studied. The incorporation of the $Eu(tta)_3(H_2O)_2$ complex in the PCL(530)/siloxane matrix resulted in a significant enhancement of the $^5D_0$ quantum efficiency (from 29.0% in the complex to 44.2% in the hybrid). The opposite situation occurred when $Eu(tta)_3$phen was added to the same medium, with the $^5D_0$ nonradiative paths in the hybrid being higher than those existing in $Eu(tta)_3$phen itself. Under UVA exposure, the emission intensity of

PCL(530)/siloxane/Eu(tta)$_3$(H_2O)$_2$ decreased 10% in 11 h, whereas that of the PCL(530)/siloxane/Eu(tta)$_3$phen decreased 25%. It is noteworthy that the thermal stability of both doped samples is remarkably high (up to 200 °C). The data derived from the present investigation lead us to state that a lanthanide aquocomplex containing β-diketonate ligands may be efficiently anchored to the PCL(530)/siloxane host network by means of the carbonyl oxygen atoms of the latter structure, which act as efficient coordinating sites toward the lanthanide ions. In the case of the Eu(tta)$_3$(H_2O)$_2$ complex, this process resulted in the release of 1 (2) water molecules from the Eu^{3+} coordination shell. When the host matrix was doped with the Eu(tta)$_3$phen complex, the absence of the labile water ligands and the presence of a strongly chelating ligand (i.e., phen) disabled the exchange of coordinating atoms (i.e., the replacement of the water oxygen atoms by the matrix carbonyl oxygen atoms). The di-ureasil hybrids with Euphen complex are luminescent hybrid materials exhibited the characteristic emission lines of Eu^{3+} ions under UV irradiation. Almost no luminescence from the host or ligand phen could be detected, indicating an efficient energy transfer from the ligand to Eu^{3+} ions. There are at least two different Eu^{3+}-local coordination sites, and the lifetime values are around 0.23 and 1.07 ms.

Sol–gel-derived KCF_3SO_3-doped di-urea cross-linked poly(oxyethylene) (POE)/siloxane (di-ureasil) ormolytes with $\infty > n \geq 1$ (n is the number of oxyethylene units per K^+ ion) have been analysed. Samples with $n > 40$ are thermally stable up to 310 ºC. At n≥100, POE crystallites are present. At n=5, a crystalline POE–KCF_3SO_3 complex with stoichiometry 1:1 is formed. In the xerogel with n=1 this complex coexists with free salt. The highest ionic conductivity is reached at n=20. The redox stability domain of this material spans 5.0 V. ‘‘Free’’ anions and weakly coordinated $CF_3SO_3^-$ ions appear to be the main charge carriers at n=20. The K^+ ions interact with the urea carbonyl oxygen atoms at all salt concentrations. Complexation of the cations by POE occurs at n=20. In the latter composition range, contact ion pairs and higher ionic aggregates develop. The ormolytes were successfully used in the assembly of prototype electrochromic devices (ECDs) that exhibit good electrochemical stability and demonstrate a memory effect. The ECD incorporating the ormolyte with n=20 displays an average transmittance in the visible region of ca. 90% in the coloured state and of 85–95 % in the bleached state. The corresponding change in colour, evaluated on the basis of the Commission Internationale d’Eclairage (CIE) colour-coordinates system, is reversible: from yellow (0.38, 0.37) for the bleached state to blue (0.29, 0.29) for the coloured state.

The energy transfer mechanisms that occur in sol-gel derived di-ureasil hybrids incorporating [Eu(btfa)$_3$(4,4′-bpy)(EtOH)] (btfa= benzoyltrifluoroacetonate, 4,4′-bpy=4,4′-bipyridine) or Eu(CF_3SO_3)$_3$ were quantitatively described. The ground state geometries were predicted by the Sparkle/AM1 model. For the hybrid incorporating [Eu(btfa)$_3$(4,4′-bpy)(EtOH)] the energy transfer rates were estimated generalizing ideas previously proposed for the intramolecular energy transfer between excited ligand levels and Eu^{3+} ions and those ligand levels and LMCT transfer states in lanthanide coordination compounds. Host-to-Eu^{3+} energy transfer occurs either via ligand excited states (essentially the triplet, T) or directly from the hybrid emitting centers through the dipole-dipole, dipole-2λ pole (λ= 2, 4, and 6) and exchange mechanisms. The ligand-to- Eu^{3+} energy transfer rate is typically 1 order of magnitude larger than the value estimated for the direct transfer from the hybrids emitting centers, 3.75×10^{10} and 3.26×10^{9} s^{-1}, respectively, to the $^5D_1$ level. The most efficient luminescence channel is (Singlet ground state, $S_0)_{Hybrid}\rightarrow(T)_{Hybrid}\rightarrow(T)_{Ligand}\rightarrow(^5D_1, ^5D_0)\rightarrow{}^7F_{0\text{-}6}$. The predicted room temperature emission quantum yield lies in excellent agreement with the corresponding experimental value (53 and 50±5%, respectively), pointing out that the Sparkle/AM1 model could, under certain conditions, can be applied to Eu^{3+}-based organic-inorganic hybrids. The Förster and Dexter classic approaches were applied to the di-ureasil doped with Eu(CF_3SO_3)$_3$. The evidence points out that the exchange (Dexter) mechanism accounted for energy transfer, namely the critical radius calculated according to the Förster model (3.3-3.5 Å) is in good agreement with the experimental Eu^{3+}/NH-C=O distance (<3.5 Å) pointing out that the D and A species have to come in contact, a

pre-condition of Dexter, for which the obtained overlap integral values are compatible. Furthermore, the calculated values for the energy transfer efficiency taking into account the Förster model are much different than the experimental ones. Therefore, although less efficient, relative to the di-ureasil containing the [Eu(btfa)$_3$(4,4′-bpy)] complex, the hybrid-to-Eu^{3+} energy transfer is also dominated by the exchange (Dexter) interaction. The detailed characterization of these energy transfer mechanisms through a quantitative assessment contributes to the recognition of the paths needed for the development of lanthanide-doped siloxane-based organic-inorganic hybrids characterized by interesting photonic features and high light emission efficiency. Moreover, the reported procedure provides a theoretical scheme that might be useful in guiding the interpretation of experimental data and in the modeling of novel organic-inorganic hybrids.
The magnetic properties of iron oxide (ferrihydrite and others) nanoparticles in organic-inorganic hybrids and polymer matrices were investigated, as well as the effects of particle size distributions on the magnetic properties/anisotropy.

C60 Phase Transitions Under High-Pressure. The structural mechanism by which C60 amorphises to carbon sp^2-phase will be addressed and new attempts to determine the structure of new carbon clathrates will be done, including complementary computer simulations.

Development of Spectroscopic Techniques. Solid-state NMR has been used has a tool to study hybrid solids. In particular, high-resolution ^{1}H NMR techniques (including Lee-Golburg based ^{1}H-^{1}H decoupling schemes such as FS-LG) were investigated in hybrid materials in tandem with other characterisation tools. Application examples of such techniques have reported for (i) yttrium-benzoate layered nanohybrids, to study the host-guest interactions, evidencing Y-O-C bondings; (ii) [La(H_3NMP)]•1.5H_2O [H_3NMP^{3-} = nitrilotris(methylenephosphonic acid)] to assign POH, P=O and NH groups; (iii) the study of amide-functionalized hybrids.
The potential of SERS (Surface-Enhanced Raman Scattering) in the study of the interaction of metal nanocrystals with molecular adsorbates was explored, in particular for the investigation of adsorption modes and orientation of molecules on the surfaces, with relevance in nanoparticle assembly studies.

Cyclodextrins. Metallocene dichlorides Cp_2MCl_2 (M = Ti, V, Nb, Mo) have attracted considerable interest due to their anti-tumour activities against a range of tumour cell lines. Following previous work where the Ti, V and Mo derivatives were encapsulated in cyclodextrins (CDs), native β-CD and TRIMEB inclusion compounds containing Cp_2NbCl_2 were prepared. A Monte Carlo optimisation run on the powder XRD pattern of microcrystalline TRIMEB·Cp_2NbCl_2 allowed us to determine that the inclusion compound crystallises in the monoclinic system with the space group P21, and a hypothetical structural model of the crystal packing was presented. The host packing and guest inclusion geometry were further confirmed by *ab initio* calculations. In another study, $CpFe(CO)_2Cl$ and $CpMo(CO)_3Cl$ were encapsulated in β-CD and TRIMEB. The Mo-containing compounds exhibited promising behaviour as catalysts for the liquid-phase epoxidation of cyclooctene. Single crystals of the TRIMEB-$CpFe(CO)_2Cl$ adduct were obtained, allowing the structure to be solved by X-ray diffraction. As part of the effort to prepare other metal carbonyl complexes (as potential guests for CDs), the complex $Mo(CO)_4$(2,2'-bipyridine) was prepared and its structure solved by single crystal X-ray diffraction.

Compounds with anti-tumoral activity may find, in general, difficulties to reach their targets, mainly due to non-compatibility with the physiological medium (hydrolysis or enzymatic inactivation) or to toxicity. Their inclusion in "safe" vehicles is a tentative way to overcome these problems. Inclusionof Ru(II)-thioether/polypirydilic complexes (previously synthesised and new ones) into cyclodextrins (CD´s) will be continued to be studied. The newly designed complexes will possess suitable ligands for *in vivo* media, such as α-aminoacids and/or organometallic fragments, which efficacy has already been demonstrated. Both new compounds and the CD´s-adducts will be characterized, in solution and in the solid state, by NMR, FTIR/Raman techniques, TG and X-ray diffraction analysis.
New inclusion systems have been obtained, resulting from the reaction of ruthenium(II)-thioether/polypirydilic complexes and several types of cyclodextrins. For the same purpose, new ruthenium(II) compounds with α-aminoacids have also been prepared.
Other research topics: (i) comparison of the aggregation processes of sodium decanoate and decanoic acid in aqueous solution (D_2O); (ii) influence of alfa- and beta-cyclodextrins and their methylated derivatives on the aggregation process of sodium decanoate. The first topic dealt with the analysis of the ^{1}H NMR chemical shift variations for the methyl protons of sodium decanoate and decanoic acid in D2O solutions using reduced variables. It was found that the recorded chemical shift variations are consonant with a narrow distribution of sizes about the mean aggregation number for decanoate ion micelles, in contrast with decanoic acid polydisperse aggregates which increase their size with concentration, until phase separation is reached. At defined temperatures between 10 and 50^{o}C, the chemical shift coefficients for the methyl group protons exhibit a negative temperature slope (shielding) for decanoate ion micelles and a positive temperature slope (deshielding) for decanoic acid aggregates. These results suggest that the increase of temperature improves the mobility of the decanoate ion chains in the micelles, thus inducing the methyl groups of the decanoate ion micelles to spend more time near the micelle–water interfaces. In turn, the size of polydisperse decanoic acid aggregates increases with temperature. The second research topic considered during 2007 aims at studying the influence of alfa- and beta-cyclodextrins and their methyl derivatives on the aggregation process of sodium decanoate in D_2O solutions. A large amount of Small Angle Neutron Scattering (SANS) data was collected at the Laboratoire Léon Brillouin, Saclay, France, and the extensive I vs Q raw data have been treated in order to be analysed.

Oxomolybdenum Catalysts. The following *cis*-dioxomolybdenum(VI) complexes were prepared and characterised by ^{1}H-NMR, IR and Raman spectroscopy, and in some cases single crystal X-ray diffraction: (a) $[MoO_2L]$ with tetradentate $[N_2(imine)O_2]$ salen-type ligands (L); (b) $[MoO_2X_2L]$ (X = Cl or $OSiPh_3$) with bidentate $[N_2(imine)]$ salen-type or pyrazolylpyridine ligands (L); (c) $[Mo_2O_4(\mu_2\text{-}O)Cl_2(pzH)_4]$ (pzH = pyrazole), with an unprecedented and extremely rare all-*cis* configuration at each of the $MoO_2(\mu_2\text{-}O)Cl(pzH)_2$ cores; (d) $K_2[Mo_2O_5(C_2O_4)_2(H_2O)_2]$. Most of these compounds were examined as catalysts for the liquid-phase epoxidation of olefins (cyclooctene, cyclododecene, 1-octene, *trans*-2-octene, (*R*)-(+)-limonene, styrene, α-pinene, *cis* and *trans*-β-methylstyrene) by *tert*-butylhydroperoxide. The oxo-bridged dimer $[Mo_2O_4(\mu_2\text{-}O)Cl_2(pzH)_4]$ exhibited excellent stability and catalytic performance for the epoxidation of cyclooctene and (*R*)-(+)-limonene in the absence of additional organic solvents, giving turnover frequencies as high as 32000 mol mol_{cat}^{-1} h^{-1} for cyclooctene epoxidation.

Chemical Modification of Electrodes With Functional Materials. Chemically modified electrodes (CMEs) were functionalised with ion-exchange polymers for the low cost, fast and direct determination of trace metals in

environmental samples. Polymer layers (micrometer thickness) were deposited on glassy carbon electrodes (GCE) by solvent evaporation. For application to trace metals, a nanometer thick layer of mercury was plated afterwards. The polyelectrolyte was poly(sodium4-styrenesulphonate). The effect of the characteristics of the PSS casting solution on the electrodes performance was analysed. Further, the mercury nanometer thick modified GCE was applied, for the first time, to determination of trace lead in recent speciation techniques such as scanned stripping chronopotentiometry.

CMEs were also functionalised with heteropolysilicotungstates (HPT) as specific materials for electrocatalysis. GCEs were modified with adsorbed single layers of hybrid salts (tetrabutylammonium, TBA) of HPT of general formula $[XW_{12}O_{39}]^{n-}$, $[XW_{11}O_{39}]^{n-}$ and $[XW_{11}M(H_2O)O_{39}]^{n-}$ (X= P,Si; M=Fe(III) and Co(II)). The electrochemistry of the immobilized hybrids was assessed, namely the redox reversibility and formal potentials as well as the effects of the solution pH on the overall behaviour. The electrochemical features of the immobilized TBA-HPT were compared with those of the same water-soluble polyanions.

ELECTROCERAMICS

Microwave Dielectric Materials. It has been found that the dielectric behaviour of (1-x)La($Mg_{1/2}Ti_{1/2}$)O_3 – xBi($Mg_{1/2}Ti_{1/2}$)O_3 and (1-y)La($Mg_{1/2}Ti_{1/2}$)O_3 – y($Na_{1/2}Bi_{1/2}$)TiO_3 with content of Bi higher than 15 mol% is mainly affected by low-temperature dielectric relaxation. This relaxation process correlates with content of bismuth in these systems and contributes to their dielectric response. The effect seems to be a universal feature of oxygen-octahedral systems with disordered Bi^{3+} cations at A-site. Anomalies of ultrasonic velocity and attenuation at the phase transitions have been observed in lead-free ceramics (1-x)$BaTiO_3$ – xLa($Mg_{1/2}Ti_{1/2}$)O_3 ($0.025 \leq x \leq 0.10$) which exhibit the continuous crossover from ferroelectric to relaxor behaviour. Particular compositions of the system were dielectrically investigated over the extended frequency range from 20 Hz to 10 GHz and the respective distribution function of the relaxation times was calculated. Dynamics of these phase transitions have been analysed and discussed.
Previous studies revealed that 52 μm-thick $BaNd_2Ti_5O_{14}$ films, with a dielectric permittivity and a loss tangent of 107 and 0.0006 (Q of 1600) at 1 MHz, respectively, and no significant increase of the loss took place up to GHz range exhibit an obvious textured microstructure characterised by grains markedly elongated. Because the microstructure of ceramics has an important impact in their final properties, the reasons for this elongated grained microstructure and its relation with the dielectric response is being studied. The impact of three effects on the anisotropic microstructure development of BNT films and thereby on the properties is under study. These effects are: 1) the electric field used for EPD, 2) the substrate and 3) the sintering temperature.
A cost effective and hazard free sol gel method for the synthesis of single phase $MgTiO_3$ thin film was established, using $(MgNO_3)_2.6H_2O$ and $TiC_{16}H_{36}O_4$ as precursors and employing either acetic acid or acetyl acetone as the stabilizers for titanium n-butoxide. The effect of the stabilizers on the structure, microstructure and electrical properties is evaluated. Acetyl acetone based films have a denser and more homogeneous microstructure than the acetic acid derived films, which is directly reflected in their dielectric properties. Acetyl acetone derived films annealed at 700 °C exhibit a dielectric constant, $\varepsilon_r = 16.3$ and dielectric loss, $\tan\delta = 0.0021$ at 1 MHz. The differences are attributed to the lower reactivity of acetyl acetone stabilized sols and higher crystallization temperature of acetyl acetone derived film.

Ferroelectric Ceramics. The microstructure evolution of textured $SrBi_2Ta_2O_9$ ceramics fabricated by template grain growth (TGG) was examined using a stereological analysis. A bimodal microstructure dominated by a large number of big anisometric grains was obtained at the final stage of the TGG process. A fast increase in the volume fraction of large anisometric grains is observed after 2 h of sintering time at 1250 ºC. The time evolution of the microstructure revealed that the number of large anisometric grains at the late stage of the TGG process is almost 4 times greater than that at the early stage. Therefore, new large anisometric grains appear in the matrix acquiring similar platelike morphology and alignment than the original seeds. It is suggested that the aligned templates induce the alignment of the small matrix grains showing a face-to-face contact, which bonded to each other to form new large anisometric grains.

Ferroelectric Fibers, Single Crystals and Films. Different macroscopic properties of PZT fibers have been obtained when using acetic acid and methacrylic acid to modify the PZT precursor. In order to clarify the role of the acids the molecular structure of the acidified PZT precursors was investigated and compared by gas chromatography-mass spectrometry, Fourier transform infrared, ^{13}C NMR spectroscopy and the reason for obtaining long PZT fibers is discussed. The results indicate that when methacrylic acid was used, long gel and ceramic fibers have been obtained because strongly co-ordinating carboxylate groups of methacrylic acid were

formed. Linear chains, like those of methacrylic acid propyl ester and methacrylic acetate, have been formed in the PZT precursor sols. In addition, after heat treatment the polymer decomposed quickly so that pure perovskite could be obtained at low temperature in the PZT fibers. When acetic acid was used short fibers were obtained. Acetic acid may act as chelate agent to form oxo acetate in the precursors; this oxo acetate nature also resulted in PZT fibers drawing. However, the longest gel and ceramic fibers have been prepared from precursors with methacrylic acid.

The fabrication and characterization of composite films comprising classical ferroelectric ($PbTiO_3$, PT) and relaxor ($PbMg_{1/3}Nb_{2/3}O_3$, PMN) material was accomplished. Thick films consisting of ferroelectric and relaxor phases in the thickness range of 2–10 mm are fabricated on Pt-coated Si substrates at a temperature of <550 ºC via a modified sol–gel route. The phase purity of the composite films was determined by XRD. The morphology and composition homogeneity were analyzed by scanning electron microscopy (SEM), energy-dispersive X-ray analysis (EDX), and by X-ray mapping method, respectively. High dielectric permittivity (e ~ 1100) and low loss values (tand ~0.03) at 1 kHz and room temperature were measured on 2 mm thick composite films for a particular composition of 83 mol% of a PT phase and 17 mol% of a PMN phase, with associated remanent polarization of P ~ 31.6 mC/cm^2 and coercive field of E_c ~ 166 kV/cm. Piezoresponse force microscopy analysis of the composite film showed that the film is piezoelectric and switchable. The temperature dependence of the effective dielectric permittivity and loss of the films at different frequencies was studied in the temperature range 50 º to 200 ºC. In the temperature range used for applications (50 º to 1100 ºC) the composite shows quite low temperature coefficient of capacitance ~18%, much lower than both PMN thick film and PT film in the same temperature range. This composition is therefore promising for low TCC applications.

$SrBi_2Nb_2O_9$ (SBN) thin films produced with SBN seeds were characterized via Rutherford Backscattering (RBS) and Particle Induced X-Ray Emission (PIXE) techniques. The obtained results demonstrated that the presence of seeds benefits the seeded film composition, as the seeded film presents lower Sr and Nb depletion as compared to the unseeded ones. The seeds effect resembles that observed for their counterpart $SrBi_2Ta_2O_9$ (SBT) thin films, i.e., the seeds behave as a barrier for the interdiffusion of the thin film and substrate elements. This work has completed the study on the preparation and properties of bismuth layered structured ferroelectric thin films which was the subject of a PhD thesis concluded in 2007.

Incipient Ferroelectrics. The dc electric-field dependence of the dielectric constant in $Sr_{1-x}Mn_xTiO_3$, x = 0.005 – 0.02 ceramics was studied in the temperature range from 10 to 125 K, i.e., around the T peak temperature T_{max}. Results were analyzed using equations derived analytically from the implicit equations of the Landau-Ginzburg-Devonshire LGD theory. Corrections due to cluster contribution attributed to the reorientation of random-field-induced polar nanometer-scale regions turn out to be important, if not decisive, for a reliable description of dielectric permittivity. So, it is found that a combined equation including the Langevin-type cluster term, is the most suited to describe the dc electric-field dependence of the dielectric constant around Tmax. Based on the fitting of the E data, the cluster polarization P_0 reaches values as high as 0.4 mC / cm^2 with the cluster size L of 11 ± 4.5 nm. Thus, the existence in the $Sr_{1-x}Mn_xTiO_3$ system of polar clusters with nanometer-scale size is consistent with permittivity data and their contribution to the permittivity at E = 0 and temperatures close to T_m is estimated to be up to 30%. In addition, besides inducing the peak in T, the formation of polar nanoregions is beneficial to the high relative electric-field tunability of the dielectric constant (70%) as well as high communication quality factor K ~10,000 under 20 kV / cm at 10 kHz.

Using electron spin resonance ESR, the lattice position and dynamic properties of Mn^{2+} ions were studied in 0.5 and 2 at. % manganese-doped $SrTiO_3$ ceramics, prepared by the conventional mixed oxide method. The measurements show that Mn^{2+} ions preferably up to 97% substitute for the Sr if the ceramics are prepared with a

deficit of Sr ions. Motional narrowing of the Mn^{2+} ESR spectrum was observed when the temperature increased from 120 to 240 – 250 K, which was explained as a manifestation of the off-center position of this ion at the Sr site. From the analysis of the ESR spectra, the activation energy E_a = 86 mV and frequency factor 1 / t0 ≈ (1 – 5)10^{13} s^{-1} for the jumping of the impurity between symmetrical off-center positions were determined. Both are in agreement with those previously derived from the dielectric relaxation. This proves that the origin of the dielectric anomaly in $SrTiO_3$: Mn is produced by the reorientation dynamics of Mn^{2+} dipoles.

The mechanisms of the effect of dopants and $P(O_2)$ on the improper ferroelastic phase transition in $SrTiO_3$ were identified. The perovskite-structured $SrTiO_3$ undergoes a cubic (Pm3m) to tetragonal (I4/mcm) transition at <108 K (T_a) associated with rotations of the O octahedra in the antiphase around the [001] direction. This phase transition gives rise to modes at the R point of the Brillouin zone in the Raman spectra and superlattice reflections at 1/2{odd–odd–odd}. The effect on T_a of La^{3+} and Mn^{2+} A-site substitution and Mn^{4+} and Mg^{2+} B-site substitution in polycrystalline $SrTiO_3$ processed in air and sintering $SrTi_{0.95}Mn_{0.05}O_{3-\delta}$ in different $P(O_2)$ has been studied using in situ Raman spectroscopy and electron diffraction. The transition temperature was raised when Mn2+ and La^{3+} were substituted for Sr^{2+} but lowered for Mn^{4+} and Mg^{2+} substitution on the Ti site. Sintering $SrTi_{0.95}Mn_{0.05}O_{3-\delta}$ in N2 reduced Ta, but sintering in O_2 had a negligible effect compared to air. It is proposed that two mechanisms are responsible for the modification of Ta: (i) the creation of oxygen vacancies by acceptor doping (Mg^{2+} ions on the Ti site) and sintering $SrTi_{0.95}Mn_{0.05}O_{3-\delta}$ in low $P(O_2)$ and (ii) adjustment of the perovskite tolerance factor (t) when, e.g., La^{3+} (1.36 Å) and Mn^{2+} (1.27 Å) substitute for Sr^{2+} (1.44 Å, decrease in t) and Mn^{4+} (0.53 Å) substitutes for Ti^{4+} (0.605 Å, increase in t).

Polar relaxation processes in lanthanum doped $SrTiO_3$ (STO) ceramics, with general formulae $Sr_{(1-1.5x)}La_xTiO_3$, were studied by undertaking field induced thermally stimulated currents measurements below room temperature. The experimental results obtained for doped ceramic (x = 0.0133) were analysed by using dipolar and space-charge relaxation thermally stimulated depolarization currents (TSDC) models in order to determine the nature of the relaxation processes involved. Our results reveal the existence of different relaxation processes in the temperature range 60–300 K. Whereas at low temperature, a relaxation mechanism of a dipolar type was disclosed within the temperature interval centered around 100 K, a space-charge relaxation process could be identified in the temperature range 120–300 K. The temperature dependence of the relaxation parameters was established.

The structure–property relations of Mg-doped $SrTiO_3$ (ST) sol–gel thin films deposited on $Pt/TiO_2/SiO_2/Si$ substrates were investigated in order to determine the effect that Mg dopants have on the dielectric properties of $SrTiO_3$. It has been predicted that Mg-doped $SrTiO_3$ should exhibit a dielectric anomaly similar to that observed recently in Bi doped $SrTiO_3$ but, to date, no polar state has been reported. It has been suggested that this may relate to the low solubility of Mg on the A-site in bulk ceramics (<0.05 at.%). However, for $Sr_{1-x}Mg_xTiO_3$ (SMT) (x < 0.30) films annealed at 750 and for SMT films annealed at 900 ºC x = 0.10, above which a Mg-rich ilmenite second phase was observed. Irrespective of the higher solid solubility limit of Mg in the ST lattice for sol–gel ST films compared to equivalent ceramics, no ferroelectric or relaxor phase transition was observed, refuting previous predictions for this dopant.

Nanoscale Properties of Ferroelectrics and Related Materials. Nanoscale fatigue properties in PZT thin films have been studied by piezoresponse force microscopy (PFM). After severe fatigue a piezoloop obtained on a fatigued point exhibits a pinched shape and a local imprint phenomenon. Domain structure evolves from a simple single-peak profile to a complex fluctuant one. Domain wall pinning and injection of electrons into the film during fatigue were suggested. The comparison of macroscopic and microscopic properties of PZT thin films with and without nano-seeds was carried out. The local piezoelectric properties of both types of films were

compared with their macroscopic electric properties. The remanent polarization values are higher in seeded films than in unseeded ones. Similarly, local piezo-response signal of single grain showed higher longitudinal piezoelectric coefficient d_{33} in seeded films than in unseeded ones. The critical voltage in which the ferroelectric domain starts to switch is lower in seeded films than in unseeded ones.

As a promising lead-free ferroelectric material, $Na_{0.5}Bi_{0.5}TiO_3$ NBT was synthesized as thin films via a classic 2-methoxyethanol sol-gel route and chemical solution deposition method. Perovskite structure with random orientation of crystallites has been obtained on platinized silicon wafer at low temperature 460 ° C. X-ray diffraction and piezoresponse force microscopy PFM have been used to analyze NBT thin films with different microstructures and properties dependent on fabrication and annealing processes. Piezoelectric activity in such films was detected.This study showed that parallel to the existence of polarization domains, some nanodomains are evidence of the lack of long-range ordering of Na+ and Bi3+ cations and seem to originate from nonuniform crystalline fields due to local fluctuations in the distribution of A-site cation composition.

Domain dynamics in the Piezoresponse Force Spectroscopy (PFS) experiment was studied using the combination of local hysteresis loop acquisition with an *in-situ* (sequential) domain imaging. The analytical theory for PFS signal from domain of arbitrary cross-section was developed, and used for the analysis of experimental data on $Pb(Zr,Ti)O_3$ polycrystalline films. The results suggest formation of oblate domain at early stage of the domain nucleation and growth, consistent with efficient screening of depolarization field within the material. The fine structure of the hysteresis loop could be related to the observed jumps in the domain geometry during domain wall propagation (nanoscale Barkhausen jumps), indicative of sufficiently strong domain-defect interactions. This was done in collaboration with Oak Ridge National Laboratory (USA).

Ferroelectric nanodomains were created in 60-nm-thick $BaTiO_3$ films using a sharp conducting tip of the scanning force microscope (SFM). The ferroelectric film, which was epitaxially grown on the $SrRuO_3$-covered (001)-oriented $SrTiO_3$ substrate by high-pressure sputtering, appeared to be single-crystalline with the (001) crystallographic orientation relative to the interface. The in-plane domain size was measured as a function of the writing time at different voltages applied between the SFM tip and the bottom electrode. It was found that the time dependence of the domain diameter deviates significantly from the logarithmic law observed earlier in $Pb(Zr_{0.2}Ti_{0.8})O_3$ films. At given writing time, the domain size increased nonlinearly with increasing applied voltage, in contrast to the linear behavior reported previously for $Pb(Zr_{0.2}Ti_{0.8})O_3$ films and $LiNbO_3$ single crystals. The dynamics of domain growth was analyzed theoretically taking into account strong inhomogeneity of external electric field in the film and the influence of bottom electrode. It was shown that the observed writing-time and voltage dependences of domain size can be explained by the domain-wall creep in the presence of random-bond disorder.

Ferroelectric domains have been investigated on the cross-section of $Pb(Zr_{0.55}Ti_{0.45})O_3$ (PZT) thin film capacitors by scanning probe microscopy. The static domain images on the cross section were obtained by lateral piezoresponse force microscopy (LPFM) method, in which the voltage used to induce converse piezoelectric effect was applied between the conductive tip and bottom electrode. The polarization-component normal to the substrate could be characterized via both d_{33} and d_{15} piezoelectric coefficients which resulted in high resolution of LPFM images. After that a variable bias was applied between the top-and bottom electrodes in order to record the variations of domain structure on the PZT cross-section. Upon the application of low bias, new domain sites appeared near PZT/Pt interface opposite to the initial polarization. Forward stretch of new domains was facilitated under dc field approaching to the coercive field E_c. Under a very high field (about three times of the E_c) the sidewise expansion of columnar domains was observed. However, the domains were only partially switched even though a very high field was applied. The observed domain growth process indicated a lower

energy barrier-for nucleation compared with that of domain wall motion. Imaginable reasons for the incomplete switching are the substantial influences of the interface and depolarization in thin film capacitors.
Local piezoresponse of individual grains in polycrystalline $Pb_{0.9125}La_{0.0975}(Zr_{0.65}Ti_{0.35})_{0.976}O_3$ (PLZT 9.75/65/35) relaxor ceramics was studied using scanning probe microscopy (SPM) technique. The observed piezoelectric contrast consisting of irregular (labyrinth-type) polarization patterns was attributed to the compositional disorder and consequent charge imbalance caused by high La concentration. A measure of this disorder, the polarization correlation length ξ, was directly determined using an autocorrelation analysis function implemented in the SPM software. The analysis of the obtained images shows that ξ taken at the scale ~200 nm varies as a function of the position inside the grain notably decreasing upon approaching the grain boundary. As a result, the average correlation length taken over the entire grain is apparently dependent on the grain size saturating at about 2 μm. The obtained dependencies are consistent with both the mechanical stress effect of impinging grains and the composition gradient in the PLZT grain and allows for better understanding of the dielectric properties of disordered ferroelectrics.
Atomic Force Microscopy (AFM) can profile surfaces at resolutions from microns to a nanometre scale. This is particularly advantageous for the studies of paper and related materials based on cellulose fibres that possess a complex structural hierarchy and constituted of major building blocks with highly dispersed dimensions, from few nanometres to tens of microns. The aim of this work was to study the morphology of cellulosic fibres from bleached *Eucalyptus globulus* kraft pulp and corresponding paper materials employing AFM technique. A series of papers was coated also with *in situ* formed silica using a sol-gel synthesis and the surface of obtained hybrid material was characterised. The dimensions and shapes of elementary cellulose fibrils, microfibrils, and macrofibrils have been determined. The diameters of elementary cellulose fibrils (4-5 nm) were of the same order as determined by X-rays scattering. The thickness of primary and secondary cell wall layers was assessed as well as the diameter and macromorphological elements of fibres. The dimensions of silica domains in the pseudo continuous film on the paper surface evidenced the mode of silica deposition in the hybrid material. This study revealed that AFM is an indispensable instrument for the study of macro- and micro- and nano substructures in the cellulose fibres and related materials.
First-principles calculations and analysis of the molecular mechanism of the polarization switching in polyvinydilene flurouride and its copolymer with trifluoroethylene [P(VDF-TrFE)] using *ab initio* quantum-chemical methods based on the HyperChem 7.52 and Gaussian-98 software were done. The simulations were performed for different copolymer contents in P(VDF-TrFE): (70:30), (60:40) and for pure PVDF. The calculated values of the dipole moment and average polarization of the molecular chains show a clear hysteresis under varying electric field with polarization saturated at ~ 0.1…0,14 C/m^2. The calculated coercive fields (corresponding to rotation of molecular chain to opposite orientation) are consistent (within the order of magnitude) with experimental data obtained on thin films (E_c=2÷10 MV/cm). In the absence of external electric field, the interactions of several molecular chains lead to the orientation of all molecular dipole moments along one parallel direction. This model corresponds to the PVDF layer on the dielectric surface. For the electric field lying in the perpendicular direction, all chains are rotated along this direction corresponding to the model of conductive substrate. Additionally developed molecular dynamic model predicts that the rotation of polymer chain provides sufficiently fast switching time (down to 10^{-12} s for thick films), while for thin films the strong electrostatic dipole interactions caused by substrate-induced and image charges lead to very long switching times (up to ~10^3 s).
In addition nanoscale piezoelectric measurements were performed on ferroelectric P(VDF-TrFE) films prepared by Langmuir-Blodgett (LB) technique. Polarization patterning, piezoelectric hysteresis and relaxation after poling are studied in this work by piezoresponse force microscopy. High quality P(VDF-TrFE) films with a

copolymer content of 30% were fabricated using a Schaefer monolayer transfer setup permitting precise control of the film microstructure. The thickness of the films deposited with 100 transfers was ~ 64 nm. Local switching resulted in the written polarization lines with the lateral size in the range 70-300 nm depending on polarization time. Local hysteresis loop (at a fixed tip position) demonstrated clear ferroelectric switching with the coercive voltage ≈ 8-10 V that corresponds to a macroscopic switching field (~1.5 MV/cm) at a ~10 nm depth below the tip. Relatively slow aging after poling was observed with the characteristic relaxation time of about 1500-2000 s depending on the polarization direction. The obtained results demonstrate that the stable polarization patterns can be created in LB P(VDF-TrFE) films and attest them as suitable candidates for memory and nanotemplate applications.

Nanoscale and Nanostructured Materials. $BaTiO_3$ crystallites with some periodic mesostructure were directly synthesised from solution via a simple sol-precipitation route. The process was of low cost, efficient and easy to be scaled up.

Multifunctional Ceramic Films and Composites. The symmetry aspects of the piezoelectric effect in various materials (single crystals, ceramics, and thin films) were overviewed. First, the third-rank tensor of piezoelectric coefficients defined in the crystallographic reference frame was discussed. On this basis, the orientation dependence of the longitudinal piezoelectric response in ferroelectric single crystals was described. This dependence is especially important for relaxor single crystals, where a giant piezoelectric effect was recently observed. Then, the effective piezoelectric constants of polydomain crystals, ceramics, and thin films and their dependence on crystal symmetry were delineated. The domain-wall contribution to the piezoelectric properties of ferroelectric ceramics and thin films was also described. Finally, the crystallographic principles of piezomagnetic, magnetoelectric, and multiferroic materials were presented.
$BiFeO_3$ is still the best multiferroic material in which the stereochemical activity of the Bi lone pairs gives rise to ferroelectric polarization, while partly filled 3d-orbitals of Fe^{3+} cause G- type antiferromagnetism. One of the possibilities to suppress the spiral spin modulation in $BiFeO_3$ is a chemical substitution in the A-sublattice. This was done in the past by doping with rare-earth ions that can themselves cause magnetic ordering at low temperatures and by using *diamagnetic* dopants: La, Sr, Pb, Ba, and Ca. Until recently, the nature of the significant enhancement of the magnetic properties of $BiFeO_3$ with diamagnetic doping was unknown. We found that heterovalent doping is accompanied by the formation of oxygen vacancies in both antiferromagnetic and weakly ferromagnetic $BiFeO_3$ thus indicating the intrinsic (i.e., not related to defects such as Fe^{2+}/Fe^{4+}) mechanism of the doping-induced magnetization. A clear correlation between the ionic radii of the substituting element and the value of the spontaneous magnetization was found. It is suggested that the biggest ionic radius ions effectively suppresses the spiral spin configuration of antiferromagnetic $BiFeO_3$. It is suggested that doping controls the magnetic anisotropy (which is known to be determined by the joint action of the anisotropic crystal field and spin-orbital interaction) via a pure structural change. Thus, A- site substitution with the biggest ionic radius ions opens up a promising way for the development of $BiFeO_3$-based multiferroics.
A series of samples of (1-x) $Y_{0.97}Sr_{0.03}MnO_3$-(x) $LuMnO_3$ system [abbreviated as (1-x) YSMO-xLMO] were prepared by a solid-state reaction method. The morphology, phase relations, and solid solution range of (1-x)YSMO-(x)LMO ceramics were then studied by x-ray diffraction and scanning electron microscopy. The results show that the single-phase ceramics with space group $P6_3cm$ is formed in the solid solution range x=0-0.30. In addition, the Rietveld refinement method was employed to study the effect of Lu doping on the crystal structure of the single-phase compositions. The lattice parameters (a, b, c and volume of the unit cell V) were decreased gradually with increasing of Lu content for these samples in the solid solution range.

MAGNETOSTRUCTURAL MODULATION OF STRONGLY CORRELATED ELECTRIC MATERIALS

***Colossal Magnetoresistive Materials*.** A main topic of study is the complex interplay of lattice structure, oxygen vacancy, defects and doping on the properties of CMR and multiferroic manganites. This leads to phase segregation at different length scales: charge or orbital ordered; insulator vs metallic. Ferroelectricity driven by magnetic order or charge/orbital order. Multiferroic hexagonal manganites: REMnO3 (RE=Er,,Lu, Eu ferroelectric) and composites (ferromagnetic/ferroelectric). Thin film preparation (sputtering) and structural studies (X-ray diffraction) for phase purity, lattice parameters and temperature study of structural phase transitions were carried out. Hyperfine local probe using implanted radioactive isotopes at ISOLDE-CERN, with Perturbed Angular Correlation Spectroscopy and Emission Channeling: to provide local and element selective information on doping mechanisms. Lattice site and electronic characterisation of the doping elements, disorder and quenched random field effects at the Mn site, in the vicinity of the charge or orbital ordered/ferromagnetic phase instability. Polaron dynamics and percolative effects in lightly doped ferromagnetic insulator manganites. Effect of charge/orbital ordering and local electrical polarization on hyperfine measurements. New field of studies started in the application of ab-initio calculations of the electronic structure and local hyperfine parameters: application to oxides.

Magnetocaloric effect and application to magnetic cooling on manganite samples as La-(Ca,Sr)MnO_3 and rare-earth (Er,Eu) doped and derived with vacancies in A and B site; effect of RE substitution on the cooling power for near-room-temperature applications. Study of magnetic entropy in competing phase systems (Ferromagnetic and charge-order). Intermetallic alloys: Pr (Ni-Co), NiMnGa and metal/metalloid Gd-Si-Ge martensitic transitions and electronic density coupled to magnetic entropy changes. Modelling of magnetocaloric properties with mean field theory. Development of experimental techniques to directly measure the magnetocaloric effect. Magnetocaloric Prototype design and development of materials.

High Temperature Superconductors. Magnetic studies of oxide superconductor materials prepared by LFZ, phase studies, critical current and their relation with structural and phase characteristics in BSCCO fibres. Magnetic and electrical studies in new MgB_2-type superconductors, superconducting fraction and critical currents. Hyperfine studies on Hg-HighTc superconductors and role of oxygen defects in fluorinated compounds.

***Other Studies*.** Magnetization and susceptibility studies on magnetic linear chain and framework silicates systems (V and Cu ions). Low-dimensionality effects: dimerization and spin-Peierls transition. Low temperature magnetic ordering and magnetic/structural modelling from Synchrotron and neutron diffraction data. Coordination systems containing magnetic ions (Co, Ni, Mn, V): crystal field effects on magnetic properties. Nanoparticle systems for biomedical applications.

REACTIVE CERAMIC COMPONENTS FOR PROCESS CONTROL

Materials For High-Temperature Electrochemical Applications. Effects of firing schedules on the transport properties of solid electrolytes have been re-examined to interpret findings which cannot be ascribed to microstructural changes. A model system ZrO_2-Y_2O_3-TiO_2 has been used to demonstrate this in fluorite-type materials and even more drastic changes were observed for pyrochlore type materials based on $Yb_2Ti_2O_7$. These effects could be ascribed to structural changes with variable sintering temperature and even on changing the rate of cooling. A proper understanding of the effects may allow optimization of solid electrolytes. Alternative spectroscopic methods (e.g. Raman and Mossbauer) were combined with refinement of XRD data, to obtain more detailed characterization of structural changes induced by changes in composition changes and/or firing schedule. Some cation conductors (e.g. $Na_{0.8}Ni_{0.6}Sb_{0.4}O_2$) were also used to study structural effects on the dynamics of ion conduction in solid electrolytes.
Reliable methods have been developed and used to characterize the onset of electronic contributions in solid electrolyte materials derived from cerias, lanthanum gallate, $Yb_2Ti_2O_7$, and silicate apatites, as a function of composition. This allows one to establish limits for the ionic domains and attempt the development of mixed conducting components for electrodes with tuned mixed transport properties dependent on the composition of the atmosphere. For new types of solid electrolytes (e.g. apatites) one examined the effects of composition changes which might be caused by interdiffusion between these electrolytes and prospective electrodes.
Several studies were dedicated to prospective electrodes for apatite-type and other solid electrolytes. Combinations of common cathode materials with apatite electrolytes show poorer performance than in combination with ceria-based, zirconia-based or lanthanum gallate-based electrolytes. $La_2(Ni,Cu)O_4$ and some alternative RP-type electrodes (e.g. $Ln_4(Ni,Fe)_3O_{10}$. with Ln=La or Pr) show interesting results for apatite electrolytes. The stability and electrocatalytic activity of these materials often depend on their oxygen stoichiometry. Pr_2NiO_4 is a very interesting model system for redox tuned phase transformation resulting in improved transport properties and enhanced electrocatalytic activity as a potential electrode under oxidizing conditions. The redox-tuning ability may also be adjusted or displaced to required temperature ranges by suitable composition changes (e.g. partial substitution of Ni by Fe or Cu). Other less common materials (e.g. $YBaCo_2O_{6-d}$) show even more complex structure-stoichiometry-property dependences. Detailed structural characterization of selected materials combines XRD refinement with lattice simulation and suitable probing methods for specific species, (e.g. Mossbauer spectroscopy for Fe, and NMR, Raman, etc., for other species).
The search for fuel electrodes included attempts to design 3-phase cermets with better resistance to microstructural ageing and to adjust the chemical nature of ceramic components for electrocatalytic purposes.
Glass compositions in the system Diopside–Ca-Tschermak clinopyroxene were investigated in order to design glass–ceramics (GCs) for SOFC sealants. The stability of the assemblage of crystalline phases over a wide temperature range (850–1000ºC) and prolonged heat treatment (up to 50 h) and the properties of produced GCs indicate high potential of these compositions for application and SOFC sealants, allowing good matching of thermal properties and strong adherence to YSZ solid electrolytes. Near stoichiometric cordierite glass-ceramic compositions **were** nucleated with TiO_2 and NiO. Heat treatment in the range 800-1200ºC yields μ-cordierite as the first crystalline phase, as found by XRD. NiO favours formation of α-cordierite.

Microstructural Effects. Nanocrystalline powders of $Ce_{1-x}Gd_xO_{2-d}$ (x=0.05-0.4) were prepared by a freeze drying method and used to prepare ceramic samples- Different grain sizes were obtaiined by changing the sintering temperature and by using cobalt nitrate ethanolic solution as sintering additive. This demonstrated that grain boundaries play a major role in the low to intermediate temperature range, especially for the lowest contents of Gd. Results also show that the sintering additive plays very important effects on grain boundary properties and allow one to approach the upper conductivity limit imposed by truly bulk properties. Similar results were obtained for other $Ce_{0.8}Ln_{0.2}O_{2-d}$ materials with Ln=La, Y, Sm. Common features to all these systems is a slight increase in a minor p-type electronic conductivity in air, and enhanced kinetics of oxygen reduction, which is probably due to the onset of mixed conductiviy in combination with active grain bounadries. Additions of Fe to $Yb_2Ti_2O_7$ also showed that suitable sintering additives may play additional positive effects on bulk and grain boundary transport properties of other ionic conductors. Other results with ceria-based materials indicate that some sintering additives may counter deletereous effects of contaminants (e.g. silica).

Mixed Conducting Materials and Catalysts for Oxygen Separation or Partial Oxidation of Hydrocarbons. Recent developments on mixed conducting membranes included detailed characterization of correlations between transport properties, redox behaviour and structural differences, characterized by refined diffraction data combined with relevant spectroscopy results and lattice simulations for selected cases. Representative examples were based on modified perovskite-type materials (e.g. $La_{1-x}Ni_{0.5}Ti_{0.5}O_{3-d}$, $La_{1-x-y}Ce_xSr_yFeO_{3-d}$ and $La_{1-x}Sr_xFe_{1-y}Nb_yO_{3-d}$), or layered materials (e.g. $Ln_2(Ni,M)O_4$ or $Ln_3(Ni,M)_2O_7$ or $Ln_4(Ni,M)_3O_{10}$ with M=Cu,Co,Fe). Very interesting mixed conducting and oxygen permeability results were also obtained for fluorite materials based on $Ce(Pr,Zr)O_{2-d}$, probably at the highest level in this structure type.
Some of the above-mentioned materials were tested in the form of flat plate configuration and under methane/air gradients to assess their aplicability in partial oxidation. Interestingly, some of these materials indicate that partial instability under strongly reducing conditions may play a positive catalytic effect, suggesting local formation of redox tuned catalysts. Other results were obtained for $SrFeO_{3-\delta}$-($SrAl_2O_4$) composites, or 2-layer dense/porous tubular membranes, based on a suitable combination of a porous $La_{0.5}Sr_{0.5}FeO_{3-\delta}$ layer and a dense $SrFeO_{3-\delta}$-($SrAl_2O_4$) layers.

Materials for Other Electrochemical Processes. $La_{1-x-y}Sr_xCo_{1-z}Al_zO_{3-\delta}$ and $La_2Ni_{1-x}Me_xO_{4+\delta}$ (Me = Co, Cu) ceramic electrodes were tested as oxygen anodes in alkaline conditions and compared with classical Ni-based anodes with hydroxide active layers. Voltametry was used to compare the electrochemical formation of those scales in both types of anodes. In addition, one used a model system of $Co(OH)_2$-$La(OH)_3$ composite films deposited onto quasi-inert metallic substrates to demonstrate the relative effects of active $Co(OH)_2$ and inert $La(OH)_3$, thus explaining the differences between $La_{1-x-y}Sr_xCo_{1-z}Al_zO_{3-\delta}$ and $La_2Ni_{1-x}Me_xO_{4+\delta}$, and also the advantages of seeking L-deficient compositions. One also found good correlation between the the electrocatalytic activity and distribution of Co^{n+} with different valence states.
Recent results showed remarkable improvement of oxygen electrodes in the presence of hematite suspension in strongly alkaline media.

***Diamond Coatings*.** Microcrystalline and nanocrystalline diamond (NCD) were growth by microwave plasma chemical vapour deposition (MPCVD), using argon rich plasmas (N90% Ar) in Ar/CH4/H2 gas mixtures. Silicon substrates were pretreated by abrasion using micrometric (~0.5 μm) and nanometric (~4 nm) diamond powders. The observed morphology evolution from nano- to microcrystalline diamond was explained by growth of crystallographically aligned construction of nanoparticles.
The bio-tribological characterization of NCD coatings on a silicon nitride ceramic biocomposite was conducted in experiments up to 500,000 cycles. Very low friction coefficients of 0.01–0.02 and wear rates of $k \sim 10^{-10}$ mm^3 $N^{-1}m^{-1}$ were measured using HBSS. For FBS lubrication larger values are due to a protein attaching effect.
Aiming at CVD diamond adhesion improvements, several electroconductive ceramic cutting tools were developed. HFCVD diamond films from nanometric to microcrystalline grain sizes were tested with Brale tip indentations. A new pilot plant size HFCVD reactor for the deposition of areas up to 25 x 25 cm^2 and another laboratory scale reactor were designed and constructed.

Other Hard and Ultra-Hard Materials. Microcrystalline diamond (MCD) grade due to its higher crystallinity and superior hardness presented the best interfacial crack resistance. CF_4 plasma pre-treatment of the substrate proved essential to maximize adhesion. Besides CVD diamond, diamond-like carbon (DLC) are also considered to be adequate coatings for tribological purposes, namely against iron alloys in automotive parts. Plasma enhanced chemical vapour deposition (PECVD) of DLC-Si or pure DLC coatings were performed, respectively, by conventional rf glow discharge from gaseous mixtures of methane and silane or taking only pure methane, with self-bias voltages varying from -200 to -800 V. An improved tribological response was obtained with pure DLC coated Si_3N_4 discs sliding against the stainless steel pins. This system almost instantaneously attains a steady-state friction regime with friction coefficients in the range 0.20–0.30 and a wear coefficient value of about $10^{-6}mm^3N^{-1}m^{-1}$, i.e., one order of magnitude lower than that of the DLC-Si coated ones.
Dense TiB_2 films, without a columnar structure, were magnetron sputtered on quenched and tempered tool steel substrates (AISI H13 premium/EN X40 CrMoV 5-1-1) as part of a project on new solutions for the aluminium injection industry.
An erosion test machine was constructed for normalized tests (ASTM G76).

Processing Methods. Ternary carbides of Ti_2AlC and Ti_3AlC_2 with laminated grain morphology were prepared by combustion synthesis.
In order to explore the high strength and hardness, good wear resistance, and excellent thermal shock resistance of SiAlON materials, rod-like α-SiAlON and of β-SiAlON powders stabilised with single and multi-cations were prepared by combustion synthesis and used as reinforcing elements of structural sialon-based ceramics densified by pressureless sintering. Mechanical activation was also successfully used to synthesise yttrium-stabilized α-SiAlON by combustion in air. SiAlON whiskers with various morphologies were produced at the surface of hot-pressed bulk samples by heat treatment at 1800ºC. Curved bow-like and kinked whiskers were also observed. The vapour–liquid–solid growth mechanism was proposed as the main growing mechanism for the whiskers.
The friction and wear behaviour of advanced structural ceramics based on SiAlONs were tested by a pin-on-disk tribometer under dry sliding conditions, at room temperature, and steel DIN-Ck45K. The results revealed excellent hardness and thermal shock resistance of the α phase. The α-SiAlON ceramics produced through colloidal processing and pressureless sintering proved to be suitable for wear resistant applications.

Titanium nitride (TiN) was prepared by combustion of Ti particles in air. The mechanism was interpreted as resulting from delayed gas infiltration behind the propagation of combustion wave. With the addition of NH_4Cl or carbon black, the yield of TiN could be enhanced. The as-synthesized TiN grains showed a terraced morphology, and this was ascribed to a surface-coarsening process.
Combustion synthesis (CS) and solid-state reaction methods were also used to prepare powders of Al_2O_3, $MgAl_2O_4$ spinel, and 20wt.% ZrO_2–$MgAl_2O_4$ and the effects of the preparation method on the sintering ability, microstructural features, and mechanical properties were investigated. The agglomerated nature of the CS powders hinders the sinterability. The agglomerated nature of ZrO_2 ceramics determines the pore and grain size distributions and thermal conductivity of porous ZrO_2 ceramics. An effective medium approach was used to model the thermal conductivity of porous ceramics.
Thermodynamic studies were carried out on AlN ceramics consolidated from aqueous suspensions after protecting the AlN powder against hydrolysis with phosphate species. Based on thermodynamic calculations and measured weight loss on heating to sintering temperature, one analysed chemical reactions occurring during firing and correlated these to density and microstructural features of AlN samples and their properties. A similar approach was used to tailor colloidal suspensions of submicron and nanosized SiC particles, coated with aluminium oxy-hydroxide to modify their electrokinetic behaviour and to act as sintering additive.

Corrosion Protection Methods. The main activity of the group during the reporting period was devoted to the different aspects of the corrosion protection for various metallic substrates. The different components of the protective system such as surface pre-treatments, anti-corrosion inhibitors, organic polymer coatings and the surface modification top layers were investigated in terms of their applicability for specific metals and alloys. The main activity of the group was focused on development of novel self-healing protective coatings. The effective development of new system with self-repair ability needs deep knowledge on the mechanisms of corrosion and corrosion inhibition. Special attention was paid to deeper mechanistic understanding of the corrosion processes on nano- and micro-scale using localized electrochemical techniques.
Self-healing coatings using nanocontainers of corrosion inhibitors were developed during 2007. In one case Layer-by-Layer assembly approach was used in order to create shell on top halloysite nanotubes filled with a corrosion inhibitor. The second approach is based on the application of Layered Double Hydroxides doped with corrosion inhibitors as “smart” anti-corrosion pigments able to provide controllable release of active substance in response to the presence of aggressive corrosive compounds.
New hybrid organosilane and the sol-gel derived nanocomposite thin films were investigated as perspective pre-treatments for aluminium alloys and magnesium alloy. The developed hybrid coatings demonstrated promising results on magnesium and aluminium alloys. Weldable primers were also studied from standpoint of active corrosion protection of galvanized steel used for automotive applications. Several organic and inorganic compounds were tested as prospective corrosion inhibitors for the aluminium and magnesium alloys.
The new experimental protocols for application of SVET/SIET techniques to investigate corrosion processes in micro-confined defects of organic coatings were suggested. Simultaneous measurement of corrosion currents, pH, oxygen concentration and concentration of metallic cations dissolved due to corrosion processes in a micro-defect were measured for the first time.

A non-destructive method to assess delamination of ceramic tiles was developed, based on ultrasonic pulse velocity measurement. It was assumed that decrease in travel velocity would indicate the presence of delamination, as sound waves travel around flat pores. One discussed the reproducibility as a potential non destructive method.

Industrial sludges derived from cutting and polishing natural stones (granite and quartzite) were characterised and incorporated in red-clay-based stoneware tiles, with up to 60–70 wt.%. The new formulations showed higher flexural strength and lower water absorption than a reference industrial product. The most significant improvements were obtained with incorporation of granite sludge. The new products fulfil the requirements of the ISO 13006 standard, group BIa (porcelain tiles).

Chromium-rich ashes derived from dangerous leather residues were incorporated as colouring and fluxing agent for industrial porcelain tile formulations. The incorporation of these wastes resulted in porcelain tiles with lower water adsorption, and higher density and bending strength. These wastes can be used to adjust the colours from cream to dark brown, depending on the contents and sintering temperature.

ZnO-containing glazes were developed, characterized and incorporated (5–8 wt.%) in hard tableware porcelain. The modified porcelains featured enhanced densification behaviour, wider maturing temperature range, better mechanical properties and whiteness, and lower shrinkage than conventional hard porcelains.

Unidirectional porous glass structures coated with a nanometer TiO_2 thin film on pore walls were successfully fabricated by freeze-drying of water-based slurry of sheet glass. The green body was subsequently sintered to produce porous glass, and then infiltrated by titanium (IV) butoxide solution, dried and calcined to generate a nanometer TiO_2 film on pore walls. It is believed that the increased surface area of present porous glass with nanometer TiO_2 has more total surface area than the TiO_2 film on glass plates is more effective for phtotocatalyst application in air or water purification.

It was shown that reaction of γ-Al_2O_3-modified Al powder with water can be used to generate hydrogen at room temperature, under atmospheric pressure. Hydration of the passive oxide film in water and in the presence of OH^- ions allows reaction of metallic Al surface with OH^- ions, yielding H_2 bubbles on reaching a critical pressure.

The rheological behaviour of fresh mortars determines the material workability, having as well great influence on the hardened product final characteristics. In this work, the rheological properties of fresh lime-based mortars were investigated. The workability of fresh mortars is affected by several parameters, namely, binder/aggregate ratio, kneading water content, type and amount of admixtures. Admixtures studied included a plasticizer, an air-entraining agent and a water-retaining agent.

Neutral and cationic porphyrins were used as photosensitizers for the photoinactivation of sewage bacteria. Two of the cationic porphyrins are highly active, even against Gram-negative bacteria, inactivating ca. 94–99.8% of these at 5 μM and after 270 min of irradiation with white light (9 mW cm^{-2}).

MACROMOLECULAR MATERIALS AND BIOREFINERIES

Novel Biomass-Derived Materials and Composites. The research on the development of novel materials based on chitosan (and chitin) was pursued. The inclusion of chitosan in paper through diffusion from solutions was continued and extended to bacterial cellulose. In order to establish the extent of this insertion, as well as the mapping of the chitosan molecules in the paper sheet and in the bacterial cellulose network, these experiments were also carried out with chitosan functionalized with fluorescent groups. The measurement of the radiance of these samples is being evaluated. Preliminary essays on the coating of paper sheets with chitosan, using a laboratory size-press, were also conducted and the properties (permeability to air, roughness, mechanical properties) of the ensuing coated papers assessed. The oxypropylation of chitosan and chitin, under heterogenous conditions was tested and the ensuing viscous polyols characterized. The determination of the OH number was carried out by ^{1}H-NMR and by the typical phthalation method. Studies on the use of these polyols as macromonomers in the synthesis of polyurethanes and polyesters are in progress. In order to clarify contradictory reports and improbable literature values, a systematic study of the surface energy of chitosan and chitin, was carried out by means of contact angles measurements, before and after different purification approaches. This investigation showed unambiguously that chitosan and chitin have surface energy comparable to those of cellulose and starch and that the much lower values reported by many authors reflected the presence of hydrophobic impurities at their surface.

The study on the controlled heterogeneous modification of cellulose substrates for the development of new functional materials was pursued. The methodologies already developed and optimized for the modification of plant cellulose fibers, namely the modification with fatty acids and fluorinated reagents, were extended to other cellulose substrates (bacterial cellulose and cellophane) and also to other natural polymers like chitosan. The reaction conditions were optimized for each substrate and the modified materials characterized as previously described. The permeability of these materials to different gases is also being assessed. The study of the modification of cellulose fibers, microcrystalline cellulose and chitosan with reagents bearing isocyanate and silane groups was also initiated. These new hybrid materials were characterized.

Composite materials made up of with fatty-acid modified cellulose fibers embedded in different polymeric matrices (e.g. polyethylene and biodegradable polyesters) were prepared. The fatty acid chain length, DS and fiber load, were considered on the preparation of these composites. Their thermal and mechanical properties are being evaluated.

An investigation on novel materials based on starch was also started. Various thermoplastic starch combinations were prepared and their properties are being evaluated. In order to increase their stability towards moisture, these materials were surface modified with reagents bearing non-apolar moieties.

A series of bisfuran (A-A) and bismaleimide (B-B) type monomers were synthesised, starting from several dicarboxylic acids and diamines respectively. The synthesis of A-B type monomers starting from aminoacid type compounds was also undertaken. Finally, trimaleimide-type monomers were also prepared. The syntheses' yields were optimized, and the products obtained characterized in detail by spectroscopic techniques. The kinetics, reversibility and equilibria of the of the Diels-Alder reaction were studied at different temperatures using both furan/maleimide model compounds and bifunctional monomers.

Studies on cellulose/inorganic particles nanocomposites was pursued, focused on cellulose/Ag, cellulose/TiO_2, cellulose/SiO_2, cellulose/ZnO and cellulose/$CaCO_3$ materials. Polymer matrix-based composites, reinforced with

some of those nanomposites were prepared using biodegradable polyesters and characterized. The functional properties (including antibacterial and photocatalytic activity) was assessed for selected materials, aiming to evaluate their potential in new bio-based functional packaging materials.
Aiming to develop new functional materials based on cellulose-silica hybrids (CSHs), series of transition metal substituted polyoxometalates (POM) have been anchored to propylamine-functionalized mesoporous silica (NH_2-silica), as a model of functionalised silica phase in CSH. These POMs include V, Co and Mn Keggin-type anions such as $[PMo_{10}V_2O_{40}]^{5-}$ ($PMo_{10}V_2$) and $[PMo_{11}VO_{40}]^{4-}$ ($PMo_{11}V$), or $[SiW_{11}Co^{II}(H_2O)O_{39}]^{6-}$ and $[SiW_{11}Mn^{III}(H_2O)O_{39}]^{5-}$, and sandwich-type anions, $[(PW_9O_{34})_2Co_4(H_2O)_2]^{10-}$ and $[(PW_9O_{34})_2Mn_4(H_2O)_2]^{10-}$. Experiments at different pH were performed for the Co and Mn substituted Keggin anions.
A patent submitted on the preparation of composites of lignocellulosic and phase-change materials was granted. Tests with shoe companies have been carried out along with basic research concerning the solid-liquid equilibrium of phase change materials poorly explored. During this year we have focused particularly on the use of fatty acids and alkylcyclohexanes as phase-change materials with their solid-liquid phase transitions being characterized.
The study of the relevant properties for the use of polymeric materials from renewable resources in food packaging was continued, focusing on the influence of the polymer structure on the gas sorption. Thermodynamic state-of-the-art models were successfully used to describe gas sorption and some fundamental phase equilibria studies were performed in order to enable a better understanding of the underlying phenomena.

Upgrading Cork and Wood Pulping by-Products. The chemical valorization of depolymerized suberin components through the synthesis of new aliphatic polyesters was continued. After preliminary studies with model systems, the polymerization of depolymerized suberin was performed by emulsion polymerization or polytransterification, using various catalysts. The corresponding polyesters, with molecular weights of a few thousand, were characterized.
A series of studies have been started towards add-value products production from wastes of pulp-and-paper industry. These cover mainly the by-products from acidic sulfite pulping (evaporation condensates and sulfite spent liquor) and some by-products from sulfate pulping (isolated kraft lignin and primary sludge fibres). The chemical composition of condensates in all evaporation effects has been examined and the scheme for the acetic acid and furfural production has been proposed. The technical and economic evaluation for the acetic acid and furfural production was accomplished. The chemical composition of spent sulfite liquor was assessed and the technological schemes for the fractionation/utilization of its components were proposed.

Wood Pulping and Bleaching. The study on the xylan retention on the pulp fibres surface during *Eucalyptus globulus* kraft pulping has been pursued. Current research was focused on the evaluation of mechanisms of xylan retention. Isolated and commercial xylans were deposited on bleached pulp and cotton linters under different conditions (temperature, time, pH and xylan concentration). The preliminary results allowed concluding on the diffusion of xylan inside cell wall. This process is intensified with the increase of xylan concentration in the solution, pH and temperature.
In addition to the polyoxometalate-laccase integrated system (PLIDS) employing polyoxometalate $[SiW_{11}V^{V}O_{40}]^{5-}$ and laccase of *Trametes versicolor* for the continuous delignification of eucalypt kraft pulp, the new bleaching system with electrochemical re-oxidation of POM have been developed and tested in bleaching of eucalypt kraft pulp.
The mechanisms of lignin oxidation with POMs were studied using monomeric model compounds. A preliminary study was done to assess the mechanism of lignin oxidation and the re-oxidation of POMs by the

electronic tongue (ET) multisensor system. A kinetic study of the oxidation of substituted phenols with either vanadium polyoxotungstate, $[\alpha\text{-}SiV^{V}W_{11}O_{40}]^{5-}$ (viz. $SiW_{11}V$), or manganese polyoxotungstate, $[\alpha\text{-}SiMn^{III}W_{11}(H_2O)O_{39}]^{5-}$ (viz. $SiW_{11}Mn$), has been carried out. The reactivity of oxidation of a series of substituted phenols by $SiW_{11}V$ has been found to correlate with the σ^+ parameter of the substituents, yielding an Okamoto-Brown ρ value (i.e., -3.1) which is coherent with the electronic requirements of a rate-determining electron-transfer route. The negligible value of the solvent kinetic isotope effect (k_H/k_D = 1.06) obtained with *p*-MeO-phenol in H_2O *vs*. D_2O solution was also in favour of a rate-determining one-electron abstraction from the substrate, followed by fast deprotonation of the intervening radical cation.

Structural Studies of Lignocellulosic Materials. The structural characterization of macromolecular components of some lignocellulosic materials (banana plant, sisal and *Paulownia*) has been carried out aiming to assess the structure–properties relationships during their chemical processing. The lignin structure in different parts of pseudo-steam from banana plant *Musa acuminata* Colla var. *Cavendish* has been studied aiming to justify the steam fractionation before the pulping applications.
A series of works have been carried out on the elucidation of structural features, such as terminal groups in xylan and its structural association with glucan, of wood hemicelluloses by ESI-MS/MS and MALDI-TOF/TOF.
The isolation and detailed structural characterization of cork hemicellulose revealed that this fraction is mainly composed of acetylated 4-*O*-methylglucoronoxylans. The chemical characterization of the phenolic fractions of cork extractives by GC-MS and LC-MS was pursued. Most phenolic components identified so far (e.g. ferulic, protocatechuic, catechin, caffeic, gallic and ellagic acid) had already been reported.
The role of several depolymerising enzymes and fungi on the detailed nanostructure of cork has been continued, with strong emphasis on the direct characterisation of the complex material by NMR and FTIR methods.

Chemical Conversion of Biomass Into Chemicals. Biomass is one of the most important renewable energy sources, alternative to crude oil. Bio-sugars obtained from the major components of plant matter (cellulose, hemicellulose, lignin and starch) by hydrolysis are the raw materials to make chemicals, consumer and industrial products, and energy from biomass. Furfural, a derivative of xylose, is of high commercial interest because it can be used for the production of a wide range of important non-petroleum-derived chemicals. We have been investigating alternative processes for the production of furfural where the traditional catalyst sulfuric acid is replaced by more environmentally friendly acid catalysts. Conventional (per)sulfated bulk zirconia, mesoporous sulfated zirconia and (per)sulfated zirconia supported on an ordered mesoporous silica, with or without aluminium incorporation, were examined as solid acid catalysts for the dehydrocyclisation of xylose into furfural. Furfural yields of up to 50% could be achieved at >90% conversion, which is better than that achievable with H_2SO_4. There is ongoing confidential work in collaboration with Merck KGaA in this field, which has been reported in a confidential study sent to this company in 2007.

Other Polymer Systems and Polymer-Based Nanocomposites. A paper published reported the first experiments on shear-induced non-isothermal crystallization kinetics of polymers and demonstrate the saturation of this process at strains that depend only on the melt temperature and polymer chemical structure, without dependence on any other processing variable.
A PhD programme on the preparation of functional polymer based nanocomposites (NCs) using *grafting from* strategies has been concluded. As regards the PhD programme on polysaccharides NCs, the preparation and characterisation of chitosan/SiO_2 films has made significant progress.

A joint (UA/TUHH) MSc thesis on the preparation of Carbon nanofibers / polyamide and the study of the mechanical properties was concluded. The results obtained were superior to those reported in the literature due to the *grafting from* strategy followed.
A joint (UA/TUHH) MSc thesis on the preparation of SiO_2 @Fe_2O_3/PANI NCs and study of the electrical properties was concluded.
One MEng thesis has been concluded on dimensional stability and permeability studies of flexible PUs. Another joint (UA/TUHH) thesis involving Weber Cimenfix on the influence of polymer ageing is finishing.
A joint (UA/AAU) MSc thesis has been started on the preparation of Carbon nanotubes /polymer via ATRP. 3 other master theses have started on: i) studies on microemulsion polymerisation using ionic liquids, (ii) studies on the reduction of VOCs in paints and (iii) the preparation of ZnO/SiO_2 /Polymer using ATRP and RAFT.

Biofuels. Biofuels activities have focused mainly on biodiesel. Our long-term aim is the enzymatic production of biodiesel using lipase from a wild-type strain of *Yarrowia lipolytica* that we have been working with during the last few years. It was shown that very high enzyme activities could be obtained in two phase media using a perfluorocarbon (PFC) to enhance the oxygen transfer rate that was identified as the limiting factor on the enzyme production. The characterization of the lipase produced was carried and a communication with this work won a prize at the European Conference of Chemical Engineering, ECCE-6 that was held in Denmark this year. To develop the production of lipase in multiphase reactors auxiliary studies of the mutual solubilities of water and PFCs had to be carried and a new equation of state, CPA-EOS, was used to describe the mutual solubilities with success.
A new approach for the production of *Yarrowia lipolytica* by extractive fermentation using ionic liquids is now under way. For this purpose a detailed characterization of the ionic liquids under study is being carried and models for the most significant properties being derived to allow the development of CAMD tools for the design of the best ionic liquids to be used in extractive fermentation. During this year the focus has been on cohesive energies, surface tensions, densities and mutual solubilities of water and ionic liquids as the fluids to be used in extractive fermentation must be water immiscible. The effect of salts on the water miscibility of ionic liquids was also addressed as fermentation media are saline solutions and the presence of salts and sugars may contribute to enhance the mutual insolubility between water and ionic liquids.
An alternative approach to the production of lipase could be on an immobilized film bioreactor. For that purpose modified polymer surfaces for the selective adhesion of *Yarrowia lipolytica* cells were developed with success.
Concerning the Characteristics and formulation of biodiesel we are particularly concerned with the water solubility on the Bx mixtures relatively to the conventional diesel fuel as the polarity of the fatty acid esters make them more hygroscopic. The CPA-EoS model was also successfully extended to the description of the water solubility in hydrocarbons. The cold flow properties of the biodiesels are also of our interest and the extension of the Predictive UNIQUAC model to the description of the SLE of systems of fatty acid esters has been attempted in collaboration with the Universities of Pau (France) and UNICAMP (Brazil).
Concerning bioalcohols, an evaluation of the COSMO-RS model to the prediction of LLE and VLE of ionic liquids and alcohols was carried. The aim is to be able to develop a tool to help in the design of the most adequate ionic liquids for liquid-liquid extraction of alcohols from fermentation media or alternatively to use them as entrainers for azeotropic distillation.

BIOMEDICAL AND BIOMIMETIC MATERIALS

Biomaterials and Biological Systems. Composites of Si-based and Si-free glasses with different polymeric matrices (PMMA, PE, SEVA, PHB, PLLA) have been developed and characterized aiming to obtain novel materials with controlled bioactive and biodegradable behaviour for application in bone medicine (regeneration, cement substitution and drug delivery systems).
All glasses and glass-ceramic compositions belong to the systems Si-Ca-P-Mg, Si-P-Ca-Mg-K_2 and Si-Na-Mg and to the Si-free system Ti-Ca-P.
Work on sol-gel synthesis of silica hybrid materials for microbial cell immobilization has been pursued.
Selected formulations were tested in accellular *in vitro* tests in simulated physiological fluids to assess their mineralization capability.
In vitro tests with MG 63 cell cultures gave the first indications that the Si-free glasses allow cell adhesion and proliferation on their surface.
*In vivo t*ests with the same glasses in powder and histological observation showed that they do not promote adverse reactions in the mouse kidneys.
The preparation and characterization of carrageenan encapsulated magnetite nanoparticles has been carried out and the stability of these particles to air oxidation determined. The rheological properties of the carrageenan matrix in the presence of magnetite and silica nanospheres have also been determined. These materials have been chemically derivatised for antibody functionalisation.
The NMR characterisation of biofluids and biological tissues has been pursued for application in the following areas: (i) study of pregnancy disorders, (ii) heart failure and diabetes incidence and (iii) detection of inborn errors in newborn babies.
The metabonomic study of ostheocarsome cells has been initiated by HR-MAS NMR, in order to establish the normal metabolic profiles of these cancer cells and then go on to study the effects of several new drugs under chemical development.
The interaction of the heme-binding proteins murine p22HBP and human SOUL with different porphyrins has been studied using NMR and fluorescence quenching. The results indicate that hSOUL may not bind via the single histidine residue as initially thought. Crystals of hSOUL have been grown and initial x-ray diffraction studies carried out. Heavy atom replacement for structure determination, via production of SeMet-hSOUL, has been started. High field NMR data has been acquired for hSOUL. Molecular modelling of the mHBP-PPIX and mHBP-hemin systems has also been started.
NMR/LC-NMR studies of amniotic fluid have identified a number of new metabolites and the conditions under which metabolomic analyses may be carried out have been identified. Initial PCA analyses indicate that foetal malformations may be able to be separated from controls.

Structural Studies of Porphyrins and Corroles. The crystalline structural details of the following highly complex porphyrins and corroles, two families of organic compounds which play a decisive role in medicine and in biological organisms, have been elucidated from X-ray diffraction studies: $C_{76}H_{83}N_5NiO_4$ (a pyrido[2,3-*b*]porphyrin obtained by the reaction of a β-amino-meso-tetraarylporphyrin with cyclic enol ether), and $C_{54}H_{17}F_{15}GaN_5O_2$, a gallium(III)(pyridine) complex of 5,10,15-tris(pentafluorophenyl)corrole-3-carbaldehyde.

Artificial Receptors for Pharmaceutical and Environmental Applications. Theoretical methods, molecular mechanics and molecular dynamics simulations were applied extensively on the design of the novel receptors. Single crystal XRD was used to characterize their complexes with metal ions and carboxylate anions. In this

context, the dioxatetraaza macrocycle [26]phen$_2$N$_4$O$_2$ incorporating two phenanthroline units, has been synthesized and its acid-base behavior evaluated. Six protonation constants were determined and the protonation sequence was established by NMR. The location of the fifth proton on the phen nitrogen was confirmed by XRD of the crystal structures of the receptor as bromide and chloride salts. The two compounds have the general molecular formula $\{(H_5[26]phen_2N_4O_2)X_n(H_2O)_{5-n}\}X_{n-1}.mH_2O$ with X = Cl, n = 3 and m = 6 and X = Br, n = 4 and m = 5.5. In the solid state, the $(H_5[26]phen_2N_4O_2)^{5+}$ cation adopts a 'horseshoe' topology with sufficient room to encapsulate three or four halogen anions through the several N–H···X hydrogen bonding interactions. Two molecules $\{(H_5[26]phen_2N_4O_2)X_n(H_2O)_{5-n}\}^{(5-n)+}$ form an interpenetrating dimeric species, which was confirmed by ESI mass spectrometry. Binding studies of the protonated macrocycle towards a wide range of the carboxylate anions, including aliphatic (ox^{2-}, mal^{2-}, suc^{2-}, cit^{3-}, cta^{3-}) and aromatic (bzc^-, $naphc^-$, $anthc^-$, $pyrc^-$, ph^{2-}, iph^{2-}, tph^{2-}, btc^{3-}) ones, were performed in water solution. The protonated $H_i[26]phen_2N_4O_2^{i+}$ receptor can uptake selectively high charged or extended aromatic carboxylate anions such as btc^{3-} and $pyrc^-$ at the pH 4.0–8.5 and < 4.0 pH range respectively, from aqueous solution containing the remaining anions as pollutants or contaminants.
This investigation was extended to other phenantroline derivative receptors [26]phen$_2$N$_4$O$_2$, [26]phen$_2$N$_6$, NMe$_2$[30]phen$_2$N$_6$ in order to evaluate the presence of additional N-H groups on the binding strength and selectivity. Further insight on the experimental findings was obtained by molecular dynamics simulations (MD) in water solution. Furthermore, the binding free energies of the last two receptors to ph^{2-}, tph^{2-} and $pyrc^-$ anions were estimated from the MD simulations using the Molecular Mechanics/Poisson-Boltzman/surface area approach (MM-PBSA). The theoretical values fit well with the experimental ones. The largest binding free energies were obtained for the anions with largest aromatic rings ($anthc^-$ and $pyrc^-$) indicating that the molecular recognition processes occurs with insertion of the anion between the two phenantroline fragments with formation of a supramolecular complex stabilized by π–π interactions and multiple N-H…O hydrogen bonds.
A perspective review on the metal complexes of cyclen and cyclam derivatives useful for medical was published in Dalton Transactions. A series of the most common chelators used in Magnetic Resonance Imaging and radiopharmaceuticals for medical diagnosis and tumour-therapy, H$_4$dota, H$_4$teta, H$_8$dotp and H$_8$tetp, is examined from a chemical point of view. Differences between 12- and 14-membered macrocyclic derivatives with methylcarboxylate and methylphosphonate pendant arms and their chelates with divalent first-series transition metal and trivalent lanthanide ions are discussed on the basis of their thermodynamic stability constants, X-ray structures and theoretical studies.

Metal Complexes of Bio-Inorganic Interest. In order to assess the mechanisms of the carcinogenicity and mutagenicity of chromium, some chromium compounds were synthesised, characterized and tested (*in vivo*).
ESI-MS and ESI-MS/MS were applied to study Ru(II)-thioether systems, namely: fragmentation mechanisms of binuclear Ru(II)-thioether systems; interactions and intercalation modes with tetramer duplexes; molecular structure elucidation and fragmentation patterns in the cases of $\{(Ru[9]aneS_3)(\alpha\text{-aminoacid})\}^+$ moieties.
Advanced spectroscopic techniques (Circular and Linear dichroism and luminescence) were applied to study the kinetics of the interaction of $\{Ru^{II}[12]aneS_4\}$ with Poly(dAdT)$_2$.

SECTION 3
Activity Plan 2008

Area 1 - Advanced Micro- and Nanostructured Materials for Communications technology
Area 2 - Advanced Materials for Industrial Applications
Area 3 - Biorefineries and Biomaterials

MULTIFUNCTIONAL MATERIALS AND ORGANIC-INORGANIC HYBRIDS

New Microporous Materials. Work on zeolitic membranes, new microporous and related materials will continue. The optimization of preparing AM-3, zeolite P, ZSM-5 and faujasite membranes will be studied in order to improve the membrane quality. New organic templates and ion liquid solvents will be carefully selected and used in this work. The isomorphous substitution and properties of obtained materials will also be studied. The applications of microporous materials as ion exchanger to remove heavy metal, such as Hg^{2+}, Cd^{2+}, in water will be studied. Catalytic properties of titanosilicates will be studied.
CH_3CH_2R and CH_2=CHR adsorption on Aluminum Methylphosphonate-α: *w*ork will continue on the separation of gas mixtures of the type CH_3CH_2R / CH_2=CHR, which are commercially important. Adsorption isotherms for these compounds will be measured and Grand Canonical Monte Carlo simulations will be performed in order to explore the potentialities of these applications and eventually to find the best conditions for gas separation.
The energy transfer dynamics in mixed lanthanide open-framework silicates, known as Ln-AV-20 materials, with the stoichiometric formula $Na_{1.08}K_{0.5}Ln_{1.14}Si_3O_{8.5}\cdot 1.78H_2O$ (Ln = Gd^{3+}, Tb^{3+}, Eu^{3+}), will be investigated using steady-state and time-resolved luminescence spectroscopy. The presence of two different Ln^{3+} environments makes the Ln-AV-20 intralayer structure intermediate between purely one-dimensional (1D) and two-dimensional (2D). This unusual dimensionality prevents modelling of energy transfer kinetics by conventional kinetic models requiring the development of a computer modelling program for the analysis of energy transfer kinetics in systems of unusual dimensions.

Mesoporous Materials. Molybdenum-functionalised ordered mesoporous silicas prepared by direct grafting of MCM-41 with the complexes $[MoO_2X_2(dimethylformamide)_2]$ (X = Cl, Br) will be characterised by various techniques including EXAFS, and examined as heterogeneous catalysts for the liquid-phase oxidation of organic compounds. The synthesis of periodic mesoporous organosilicas containing organometallic groups as an integral part of the structure will also be undertaken. The organometallic fragments will be introduced by either one-step hydrolytic polycondensation methods or post-synthesis derivatisation. Luminescent mesostructured materials will be prepared by incorporation of Eu^{3+} β-diketonate complexes inside the channels of MCM-41 via a noncovalent host-guest interaction or via complexation with surface-anchored pyridine ligands. The immobilisation of these complexes in MCM-41 can improve their photostability under UV radiation and enhance the ligand-to-metal energy transfer, increasing, therefore, the emission quantum yield.
MCM-48 aluminosilicates with different Al contents will be synthesised by a room temperature procedure using tetraethoxysilane and aluminium sulfate, isopropoxide or tert-butoxide as metal sources. The catalytic activity of the samples will be tested in the reaction of 1-butene double bond position isomerisation. The influence of the synthesis time and calcination conditions, such as heating rate and time at final temperature, on the structural and catalytic properties of the materials will also be evaluated.

Layered Materials. Layered double hydroxides (LDHs) are a rare example of inorganic layered compounds with positively charged layers compensated by intercalated anions. The anions are exchangeable, giving rise to a rich intercalation chemistry. Building on previous work carried out at CICECO, the preparation of multifunctional

nanocomposite materials through the intercalation of organic and metallo-organic species into LDHs will be investigated. A range of guest species will be studied, including anionic pyrene derivatives and metal complexes of organic ligands such as heterocyclic amines, catecholates and citrate. A combination of physical methods such as powder X-ray diffraction, EXAFS and fluorescence spectroscopy will be used to provide a detailed picture of the structures of the nanocomposites, their thermal stability, and the nature of the host-guest and guest-guest interactions. Selected materials will be tested as catalysts for the oxidation of organic compounds.
The first examples of nanoparticles of pure layered $Ln_2(SiO_4H)(OH)_2(H_2O)Cl$, Ln= Eu, Gd, and Tb, and mixed microcrystalline layered Ln silicates containing different Eu/Gd and Tb/Gd ratios, will reported. Their crystal structure has been solved from synchrotron powder X-ray diffraction data. These materials display efficient and tuneable photoluminescence properties, such as energy transfer between different Ln^{3+} centres, illustrated here with the pairs Gd^{3+}/Eu^{3+} and Gd^{3+}/Tb^{3+}. Moreover, they are promising materials for sensing (at least) Cl- and F-anions.
$Zn,Al–CO_3$ compounds with the hydrotalcite-like structure will be prepared by a co-precipitation method followed by hydrothermal treatment under microwave irradiation. The influence of the ageing treatment will be studied in two series of samples with different Zn^{2+}/Al^{3+} ratios, namely, 3/1 and 2/1. Moreover, the effects of the heating temperature and of the irradiation time will be studied in order to select the optimum preparation conditions.

Nanostructured Materials. We intend to direct the work regarding the manipulation of various nanocrystals (NC) at the surface of In-containing Nitride heterostructures towards the nano-bio interface. We would like to exploit this integration platform to test and develop lab-on-a-chip device concepts related to nanomedicine. We will also extend our work on the theoretical modelling of basic material properties at the nanoscale. In particular work is in progress to model thermal conductivity and melting temperature in technologically relevant semiconductor nanomaterials. We will continue to apply and develop high-resolution X-ray diffraction methods to the characterization of advanced materials.
Ordered nanocrystalline hybrid structures will be characterized by means of scanning electron microscopy (SEM), transmission electron microscopy (TEM) and electron energy loss spectrometry (EELS). Structural characterization and the investigation of dopant distribution will guide the synthesis and modification of the inorganic and organic parts. By this we expect to add new functionalities to these materials. Furthermore, other kind of luminescent inorganic nanoparticles will be studied. Lanthanide doped strontium and barium aluminates which were recently synthesized will be the scope of advanced optical investigations.
The work on ordered nanocrystalline hybrid structures will continue especially by targeting new inorganic materials (e.g. phosphates), intercalating new organic moieties, performing advanced structural and optical characterization techniques. By changing the inorganic and organic parts we expect to add new functionalities to these materials. Furthermore, other kind of luminescent inorganic nanoparticles already synthesized by similar methods will be studied. Lanthanide doped strontium and barium aluminates which were recently synthesized will be the scope of advanced optical investigations.
The synthesis of polymer based nanocomposites containing inorganic nanocrystals will continue having in mind the study of their optical and magnetic properties. Processes of surface modification of both the nanocrystals and the composites derivatives will be investigated. In particular, we wish to investigate the development of new properties that might arise due to the interaction of the nanocrystals and the matrices used in the synthesis of the nanocomposites.

Non-Aqueous Chemistry Applied to Atomic Layer Deposition. A new non-aqueous sol-gel approach applied to the atomic layer deposition technique will be further investigated in order to synthesize multiferroic materials deposited on different substrates. Such a novel approach already brought several advantages compared to ordinary deposition and will permit to develop a new approach toward multiferroic materials. The deposited films will be characterized in terms of film thickness, crystallinity, interface thickness and atomic gradients across the interface. In addition, vanadium oxide deposited on high surface area supports will be characterized before and after catalytic reaction.

Polyoxometalates. The synthesis by several synthetic procedures and the study of new hybrid compounds with polyoxometalates (POMs) and organic aromatic moieties, either as cationic species or incorporated in metal complexes, will be continued. The obtained compounds will be assessed for their electrochemical or optical properties. Solid-solid solvent free reactions will be extended to the incorporation of inorganic cations (namely group 2 or lanthanide cations) in salts with Keggin polyoxometalates. Studies on homogeneous catalysis will be continued with new substrates. The studies on the preparation of supported transition metal-substituted polyoxotungstates, to be evaluated as oxidative heterogeneous catalysts, will be continued.Research will be continued on the preparation of new organic-inorganic hybrid coordination compounds containing lanthanides, POMs and an organic ligand. The effects of the organic ligand and the POMs on the luminescent properties will be investigated in particular, considering the possibility that they might act as sensitizers of the lanthanide luminescence. The application of the compounds in the preparation of POM based materials will be explored, namely by the preparation of mono or multilayered nanostructured films, incorporation into nanosized SiO_2 and preparation of polyoxometalate-anion-pillared layered double hydroxides.

Crystal Engineering of Organic-Inorganic Hybrids. Highly flexible organic ligands based on chelating polyphosphonic acid groups (such as etidronic acid, H_4hedp) will used in conjunction with lanthanide and transition metal centres to form novel multi-dimensional metal-organic frameworks: $Na_2[Y(hedp)(H_2O)_{0.67}]$ and $Na_4[Ln_2(hedp)_2(H_2O)_2]\cdot nH_2O$ (Ln = La, Ce, Nd, Eu, Gd, Tb, Er) (3D materials); $[Eu(H_2hedp)(H_2O)_2]\cdot H_2O$, $Na_{0.9}[Nd_{0.9}Ge_{0.10}(Hhedp)(H_2O)_2]$, $[Ln(H_2hedp)(H_2O)]\cdot 3H_2O$ (Ln = Y, Tb) and $[Yb(H_2hedp)]\cdot H_2O$ (2D materials); $M_4[M_{12}V_{24}O_{24}(OH)_8(H_2hedp)_8(Hhedp)_{16}(H_2O)_{64+n}]\cdot 88+y(H_2O)$ where M = Y, Ce and Er. The structure of these compounds will be elucidated using single-crystal X-ray diffraction, and their photoluminescent properties investigated. The obtained materials will be further studied using other more common techniques, such as conventional powder X-ray diffraction studies, TGA, SEM, EDS, FT-IR and FT-Raman and also elemental composition (CHN and metal content from ICP analysis). Efforts will also be focused at the isolation of novel complex-based crystalline compounds containing Ge^{4+} centres, in particular: $X\cdot[Ge(OH)_2(C_2O_4)_2]\cdot n(H_2O)$ [$X = C_4H_{12}N_2^{2+}$ (H_2pipz^{2+}) and n = 1; $X = C_{10}H_{10}N_2^{2+}$ (H_2bipy^{2+}) and n = 2]; $(Hbipy)_2[Ge(C_2O_4)_3]$ and $(Hphen)_2[Ge(C_2O_4)_3]\cdot 2(H_2O)$ ($Hbipy^+$ is the 2,2'-bipyridinium cation, and $Hphen^+$ is the 1,10'-phenathrolinium cation).

Porous metal–organic framework materials are important owing to their potential applications as sensors. We wil report a new family of nanoporous, multifunctional rare-earth metal–organic materials displays emission quantum yields and efficiencies that are the highest reported for solid-state Eu^{3+} compounds with organic ligands and magnetic properties.

Organic-Inorganic Hybrids Lacking Activating Centers. New functional hybrids hierarchically ordered, with potential applications in integrated optics devices, will be studied. The mechanism of the hybrids self-organization and the relationship between the ordered nanostructures and the emission properties, will be investigated.

New Hybrid Materials. Multifunctional nanohybrids, combining lanthanide luminescence property and other functions such as magnetism or biologic activity, will be studied. These multifunctional architectures are built on the core-shell structure with the functional components inside the core or covalently linked on the surface of the shell. The modified Stöber method will be used to prepare the silica particles with different sizes containing one functional component and sol-gel process or layer-by-layer assembly technique will be employed to graft another active component. The hydrophilic or hydrophobic of the nanohybrids will be modulated by introducing different groups in order to satisfy different functions.
With the goal of enhancing the photoluminescence features and the chemical stability under ultraviolet (UV) radiation exposure, different lanthanide based complexes will be incorporated in o innovative organic/inorganic hybrid matrix built from the cocondensation of two di-ureasils frameworks. The effective interaction between the lanthanide ions and the host hybrid structure, the emission overall quantum yield and the $^5D_0$ quantum efficiency will be estimated and compared with those of the isolated complexes.
The magnetic and structural properties of organic-inorganic nanostructured hybrids or polymer matrices incorporating Fe-based nanoparticles, nanoparticles, linear chains, and framework systems. will continue. The effects of inhomogeneous distributions of nanoparticle systems will be also addressed.

***Integrated Optical Devices*.** Development of innovative organic-inorganic hybrids, such as di-ureasils modified by of zirconium (IV) n-propoxide (ZPO) stabilized with methacrylic acid (McOH) to produce cost effective integrated optics devices. Investigation of the influence of the ZPO concentration, ZPO/McOH ratio, and processing method (thin films and monoliths) on the optical features. Production of enabling solutions for access optical networks, such as low cost optical power splitters and optical filters, through UV patterning of the prepared hybrids.

C60 Phase Transitions Under High-Pressure. The structural mechanism by which C60 amorphises to carbon sp2-phase will be addressed and new attempts to determine the structure of new carbon clathrates will be done, including complementary computer simulations.

Development of Spectroscopic Techniques. Probing the local environment of ^1H nuclei is an important issue in materials science. Because ^1H MAS spectra suffer from low resolution because of strong ^1H homonuclear couplings, relevant ^1H chemical information, such as intermolecular interactions, may only be obtained using certain high-resolution ^1H MAS techniques. Thus, the use of very recently developments on high-resolution ^1H CRAMPS NMR techniques, such as windowed (wPMLG-n) and windowless (SAM3) acquisition schemes, are underway. Several examples of complex hybrid materials are being used to test such NMR techniques, revealing exceptional results.
In parallel with technical NMR improvements, advanced characterization studies on hybrid materials will continue in Aveiro. However, a new family of biomimetic/bio-inspired materials based on metal-aminoacid chiral frameworks, successfully synthesized in Aveiro, will be one of the main focuses of study in 2008. The study of such bio-inspired materials by NMR and diffraction techniques is also underway. In addition to solid-state NMR, and diffraction techniques, quantum mechanical computation of ^1H NMR chemical shifts will be

employed for the first time using DFT calculations based on the use of the GIPAW approach (using plane waves basis set). Such strategy is underway and will contribute to increase the knowledge on the nature of intermolecular interactions, such as hydrogen-bonding networks and p-pstacking effects, allowing the elucidation of subtle details in the structure of hybrid materials. Therefore, DFT calculation will be an important piece to join our advanced characterization studies Aveiro.
The potential of SERS (Surface-Enhanced Raman Scattering) in the study of the interaction of metal nanocrystals with molecular adsorbates will be continued, in particular for the investigation of adsorption modes and orientation of molecules on the surfaces, with relevance in heterogeneous catalysis and nanoparticle assembly studies.

Cyclodextrins. Studies on cyclodextrins (CDs) as second sphere ligands for organometallic compounds with interesting luminescence properties or biological chemistry will continue. Heptakis(2,3,6-tris-*O*-methyl)-β-cyclodextrin (TRIMEB) inclusion compounds of Eu^{3+} β-diketonate complexes will be prepared and characterised by powder XRD, TGA and photoluminescence spectroscopy. The compounds will be tested as emissive layers in organic light emitting devices. The electrical insulating and protective properties of the CD should help to increase the durability of the device, which is usually compromised through oxidation or electrical wearing.
The study of the influence of alfa- and beta-cyclodextrins and their methyl derivatives on the aggregation process of sodium decanoate in D_2O solutions is expected to be completed. This research study combines 1H NMR chemical shift variations for the alkyl protons of decanoate ion and I vs Q SANS data in order to assess the influence of the cyclodextrins and their methyl derivatives on the aggregation process of sodium decanoate in D_2O solutions.
Ruthenium compounds will be tested as novel antitumoral drugs, either free or CD-encapsulated. Their activity will be further increased by resource to biomimetic design. Using a strategy that has proven effective, aminoacid-bearing ruthenium compounds will be prepared, encapsulated in different hosts and characterised by various solid-state techniques. Where possible, powder XRD data will be analysed to produce hypothetical structural models for the crystal packing, and data collected with synchrotron radiation may allow full refinements of the structural models to be performed. These studies will be complemented by carrying out *ab initio* calculations to elucidate preferential organometallic-cyclodextrin inclusion geometries. Finally, in an extension of previous work, heptakis-2,6-di-*O*-methyl-β-CD (DIMEB) encapsulation of $[CpMo(NCMe)_2(CO)_2](BF_4)$ and [CpMo(2,2'-biimidazole)$(CO)_2$](BF_4), and β-CD/TRIMEB encapsulation of the biomimetic complex $Mo(\eta^3\text{-}C_3H_5)$CpCOO-Phen-CH_3 (Phen = Phenylalanine) and its precursor $Mo(\eta^3\text{-}C_3H_5)$CpCOOH, will be performed. The cytotoxic and antiproliferative activity of these compounds will be screened using mouse carcinoma cell lines and the most promising compounds will be tested in human tumoral cell lines.

Chemical Modification of Electrodes With Functional Materials. The study of adsorbed films of polymers functionalized with ion-exchange groups will proceed. Cross-linking or grafting procedures with different polymers will be exploited in order to produce polyelectrolyte layers of increased concentration of ion-exchange groups of lower thicknesses. The chemically modified electrodes (CME) will be prepared by solvent evaporation on glassy carbon and their morphologic, structural, ion-exchange and perm-selective features will be assessed. The CME presenting the best performance for the determination of trace metals will be tested in direct voltammetry or in scanned chronopotentiometry.
Work will continue on the use of heteropolytungstates (HPTs) as electrode modifiers. Layer-by-layer assembled electrodes will be prepared on glassy carbon substrates using polyelectrolytes as builders. Similar assemblies will be prepared also on quartz plates, suitable for spectroscopic analysis. Other approaches will include the

preparation of composite materials incorporating the HTP species and polymer/carbon-based mixtures (carbon nanotubes/graphite, plus mineral oil/ionic liquid as homogenisers. The electrochemical characteristics of the enclosed HPT will be studied as well as the stability and morphological features. Comparison of the behaviour of the developed HTP modified electrodes with that of HTP immobilised in other environments and with that of the corresponding water-soluble anions will be made. Application to the heterogeneous catalysis of some reactions will be tested, e.g., nitrite reduction, oxygen peroxide reduction or dopamine oxidation.

Microwave Dielectric Materials. It has been recently revealed that some *A*-site deficient perovskite ceramics based on niobium and tantalum are of potential interest for microwave applications. Room-temperature values of their dielectric constant were found to be unexpectedly high, a feature not usually inherent to oxide non-ferroelectric perovskites. Moreover, the dielectric response of these ceramics is frequency-dependent at low temperatures, although no sign of a ferroelectric relaxor polar order is observed. The microwave dielectric characteristics (permittivity, thermostability coefficient and quality factor) of these niobates and tantalates at room temperature are very comparable with those of the well-known incipient ferroelectrics: $SrTiO_3$ and $CaTiO_3$. Thus the *A*-site deficient perovskites, due to their simple composition and structure, can be considered as models to study structure–property relations in microwave dielectrics. At the same time, neither crystal structure of these compositions below room temperature nor their respective dielectric behaviour has been reported before. Therefore, the crystal structure studies along with the dielectric measurements over a wide frequency range from room temperature down to 10 K are planned aiming to associate the observed low-temperature dielectric anomalies with likely structure transformations. In order to estimate the lattice contribution to the permittivity and loss of these compositions, far infrared spectroscopy studies will be also performed.
The work on the preparation of thick dielectric films by EPD for MW applications will include the following aspects: 1) investigation of the effect of different solvents on the EPD of BNT dielectric thick films with optimal dielectric properties; ii) assessement of the dielectric properties of some BNT films at MW frequencies; iii) preparation of BNT films by EPD on Al_2O_3 substrates.
For telecommunication applications such as microwave filters and oscillators, $MgTiO_3$ is reported to be ideal, due to its high quality factor (Q above 20,000 at 8GHz). However its temperature coefficient of resonant frequency, τ_f is negative (-55 ppm/^{o}C) and needs to be tuned for applications in thermostable devices. In thin films, such a tuning effect could be achieved by using a multilayering approach, in which layers of $MgTiO_3$ will be intercalated with layers of a compatible material with positive coefficient of resonant frequency. However, not all materials except $CaTiO_3$, and $SrTiO_3$ could be used for this practical purpose due to the necessary structural, chemical and physical compatibility, to avoid undesirable strains or chemical reactions, which may cause the formation of secondary phases and defects and deteriorate the Q value. Multilayering of low loss dielectrics with comparable thermal expansion and opposite temperature coefficients of resonant frequency materials could also serve as an additional means to downsize the devices. The potential application of $SrTiO_3$ layers as a ´temperature compensator´ has not been studied before. In this perspective, the possibility of using $SrTiO_3$ as a functional layers in $MgTiO_3$ / $SrTiO_3$ composite thin films, will be explore. The dielectric response of these structures will analysed at room temperature and preliminary at RF frequencies.

Ferroelectric Ceramics and Ferroelectric Fibers, Single Crystals and Films. The study of the alteration of sintering PZT thick films on Cu foil by using of different sintering aids and in inert atmosphere will be continued. Different sintering aids compositions, namely low melting point glass, lead oxide plus boron oxide, lead oxide plus vanadium oxide, will be studied as sintering aids for EPD of PZT film on Cu. The addition of sintering aids altered the feasibility EPD. The effect of concentration and molar ratio between sintering aids and PZT on the microstructure development and electrical properties of PZT thick film will be evaluated.
Novel Aurivillius oxides for microelectronics applications will be prepared and of the properties of bismuth layer structured ferroelectrics compounds with n greater than 5 (n=number of perovskite layers interleaved between bismuth oxide layers) will be analised. Bulk and thin films will be produced using the conventional oxides mixture and the sol-gel procedure. The necessary experimental conditions will be exploited so as to optimize the

preparation processes. The electrical properties of the obtained materials (bulk and thin films) will be characterized and compared.
Dielectric and ferroelectric properties of high T_c $xBiScO_3$ – (1-x) $PbTiO_3$ (BS-PT) thin films deposited on platinized and oxide electroded silicon substrates will be carried out by sol-gel. A $PbTiO_3$ seed layer or buffer layer will be introduced. The influence of $PbTiO_3$ seed layer on the electric properties and the relation with the phase formation process, crystallinity, and microstructure of the films will be discussed. Preliminary investigations will be conducted on the effect of different electrodes on dielectric and ferroelectric properties and fatigue endurance of BS-PT thin films.
$CaCu_3Ti_4O_{12}$ (CCTO) ceramics and films with high dielectric constant and low loss will be prepared by the sol–gel process and sintered at different temperature and times. The influence of sintering time on the values of the dielectric constant and nonlinear coefficient of ceramics will be studied towards tailored dielectric constant and nonlinear coefficient for specific device applications. The influence of different solvents on the phase composition, microstructure, dielectric and nonlinear properties of CCTO thin films will be analyzed and discussed. The current–voltage characteristics and Cole–Cole plots in a broad temperature range (60–400 K) of CCTO will be studied.
Composite materials with sensing capabilities that can provide the information on their current condition constitute an important class of smart materials and are in high demand for in-process and health monitoring. In-process monitoring, in situ sensors are used to control cure degree, pressure, temperature, voids, defects and residual stress in real time. This is highly needed for the optimisation of curing cycles and quality assurance. Health monitoring systems using integrated sensors provide us in situ monitoring of stress, strains and damages. Miniature sensing systems are required that could be bounded into a material without disrupting its structural integrity. Recently, optic fibres and piezoelectric ceramic fibres have become preferable stress and/or temperature-sensing elements combining small size, high sensitivity and high frequency response. However, their main drawback is a high cost of signal demodulation systems and the need of intimate bounding either at external surface or composite laminates limiting the number of sensors that can be deployed. Large-scale applications in civil structures require the development of innovative distributed sensors concepts. This can be achieved by incorporating an additional active phase into the composite matrix during initial build or retrofit. Novel sensory composites with embedded magnetoimpedance wires showing large change in electrical impedance or polarisation with respect to mechanical stress at MHz and GHz frequency bands, will be studied.

Incipient Ferroelectrics. The work within incipient ferroelectric ceramics will continue along the following lines: i) The effect of a dc and ac field on the dielectric constant and loss of $Sr_{1-1.5x}Y_xTiO_3$ (x = 0, 0.005, 0.010, and 0.016) ceramics will studied in a wide temperature range Cycle curves of the dielectric permittivity versus dc bias field and of the polarization versus ac electric field are analyzed. The probable mechanisms of induction of polar states in Y-doped strontium titanate ceramics will be studied and discussed; ii) the study of the structural properties and microstructure development of Sc-doped strontium titanate (ST) ceramics, synthesised by solid state reaction, according to the composition $Sr_{1-1.5x}Sc_xTiO_3$ with x = 0 - 0.01, will be studied. The dielectric properties will be evaluated as a function of the temperature and frequency in the radio frequency range and iii) The study of the magnetic properties of Mn doped ST ceramics in collaboration with the University of Duisburg na Alemanha.
The work within incipient ferroelectric ceramics will continue along the following lines: i) continuation of the studies on the effect of stresses induced by the substrates on the incipient response of undoped ST, ii) studies on the dc field dependence of low-temperature dielectric permittivity ε' of $SrTiO_3$ films with Mg incorporation on Sr

and Ti sites and iii) initiation of the preparation by RF magnetron sputtering thin films based on KTM (1-x)-($KTaO_3$)-x($MTaO_3$) systems.

NanoscaleProperties of Frroelectrics and Related Materials. During the year 2008, the investigations of the local properties of ferroelectric thin films, single crystals and ceramics will be extended into various materials including also PZT single crystals and films, lead-free materials, and structures based on them (PMN/PT, BTZ/BZ etc). Polarization patterns prepared by nanolithography will be studied in terms of their stability as a function of time and temperature. The domain wall motion studies (creep and activation mechanisms) will continued in other materials than PZT. The Labview programs to acquire piezoelectric signal will be modified to measure additional parameters (such as coercive voltage). The switching spectroscopy technique will be mastered.
The studies on ferroelectric relaxors including non-traditional relaxors: lead-free and artifical ones based on multilayers will continue. It is also planned to investigate solid solutions of relaxors and normal ferroelectrics to understand their high performance. This work will be correlated with the EC-funded project "Multiceal". The work will be done in collaboration with Shanghai Institute of Ceramics and Jozef Stefan Institute. The comparison with the results of macroscopic measurements will allow to reveal valuable information on the nature of relaxor state. The study will be extended into the smallest domains created by nature using liquid measurement cell available in the new setup.

Nanoscale and Nanostructured Materials. Polarization-induced assembly will be studied in several materials included selected phospho- and glycolipids. Thus obtained complex self-assembled nanostructures will be investigated by a variety of analytical and spectroscopic techniques including macroscopic (dielectric constant, polarization, switching current, pyrocoefficient, optical spectroscopy, exoelectron emission, XPS, etc) and local ones (electric potential, charge, electric field, conductivity, piezoresponse). The switching and recognition phenomena related with the dynamics of ferroelectric domains during application of external electric field will be also studied. The work will be done in a close collaboration with the University of Saarbruecken, Institute of Crystallography (Moscow), University of Riga (Latvia) and Institute of Mathematical Problems of Biology (Moscow region).
Work will continue on fabrication, structural and morphological characterization of anisotropic ferroelectric, piezoelectric and quantum paraelectric perovskites nanostructures. Identification will be attempted of the optimal processing conditions, thermodynamics and kinetics for the hydrothermal synthesis of each crystallographic phase in certain 1D morphology. The fabrication of 1D $BaTiO_3$ nanomaterials via polymer-assisted hydrothermal synthesis will be studied. Thermodynamic and kinetic models will be drawn to describe the barium titanate crystallization taking into account the anisotropic growth. Based on these models carbon nanotubes (CNTs) will be used as templates for the preparation of barium titanate 1D nanostructures.
The investigations on the preparation of mesoporous perovkites with different compositions, as powders or films in order to study of the ferroelectric properties will be pursed.
AFM analysis of hybrid nanostructure and nano-materials to the application of biomedical and microbiologic systems will be continued.

Multifunctional Ceramic Films and Composites. $BiFeO_3/BaTiO_3$ multilayers will be studied to reveal the self-doping effect. This work will be done in a close collaboration with Cambridge University, University of Duisburg-Essen, CNRS, French defense agency ONERA, several Universities and research organizations in France, Slovenia and Lithuania.

Novel composites such as PZN-PT/Terfenol D will be sintered and investigated.
Novel composite thick film materials (Ni_2FeO_4/PZT) will be fabricated by using hybrid sol-gel method. Preparation by sol-gel and characterization of magnetic powders (BiFeO/BiMnO). The processing conditions will be modified to get the right phase, to reduce the particle size, and to prevent their agglomeration for further use in multiferroic composites. Deposition of hybrid composite films: the work will be concentrated on the deposition of multiferroic films based on the obtained NiFeO, BiFeO/BiMnO powder and piezoelectric sol-gel solution (PZT, KNN). PZT sol-gel precursor solution will be optimized in order to avoid the use of highly toxic methoxyethanol route. KNN solution will be prepared using the technology transferred from the Jozef Stephan Institute (Slovenia). The work will be focused on finding optimum deposition conditions (concentration of magnetic powder, spinning speed, number of layers) and the drying and firing conditions. Further work will be done on reducing the porosity of the films and finding the way of reducing conductivity.

MAGNETOSTRUCTURAL MODULATION OF STRONGLY CORRELATED ELECTRIC MATERIALS

Advanced Materials

a) Magnetic and structural properties of: metal-organic and inorganic materials, nanostructured organic-inorganic hybrids, coordination polymers, nanoparticles, linear chains, transiton metals and rare-earth cluster compounds and framework systems.

- Iron oxide nanoparticles (maghemite, magnetite and ferritin): high magnetic field studies in ferritin, to study the antiferromagnetic component and crystal field effects on magnetic properties and magneto-structural coupling.
- Linear chain compounds with s=1/2 copper ions and dimmers/trimer cluster associations. Mixed Fe-V ferrimagnetic clusters.
- Multifunctional magnetic nanoparticles, for biomedical applications (development of magneto-optical functionalities)

b) Magnetic materials for quantum computation

Study of thermal entanglement in magnetic materials for applications in Quantum Information and Quantum Computation. Design of materials (those with transition metals chain/cluster) with quantum entanglement at high/room temperature, based on previous knowledge of magnetic behaviour of materials. Conections of thermal entanglement with strucutural properties. Possible aplication in solid-state quantum chips. Connections with Tsallis non-extensivity.

c) Models on molecular magnetism

Development of magnetic hamiltonians to understand the microscopic mechanisms that rule the magnetic behavior of linear chains and cluster compounds. Application to S=1/2 and higher cases

d) Effects of inhomogeneous distributions on the properties of nanoparticle systems

A method has been developed to analyse in a consistent way the dependence of magnetic properties on the nanoparticle size: application to ferrihydrite and other oxides already successful. It is based on a statistical nonparametric method.

Strongly Correlated Electron Systems: Theory and Experiment

a) Colossal magnetoresistive, multiferroic materials and their magneto-electro-elastic coupling effects

- Thin film preparation with RF sputtering deposition system: structural (X-ray), magnetic and electrical properties. Systems studied: La-Sr and La-Ba manganites with highest Tc (above roomtemperature) and multiferroic structures LaSrMnO3-REMnO3, BaTiO3-LaBaMnO3. ZnO thin films. Also study of growth of MgO as dielectric layers for electronic applications and buffer layer in metal-oxide structures.
- Hyperfine studies using implanted radioactive isotopes at ISOLDE-CERN. This is part of an international project in CERN. Hyperfine techniques, addressing charge/orbital order and electronic phase segregated systems; competition and interface effects; measurements of electric field gradient and hyperfine magnetic field in magnetic oxides.
- Multiferroic oxide materials: hexagonal manganites REMnO3 (RE=Er,Gd,Lu,…) and composites (Perovskite/Ferrite). Study of structural, magnetic and electrical properties; Raman spectroscopy.

-Multiferroic structures: bilayer/multilayer systems of magnetic shape-memory /ferroelectrics. Work in the collaboration MULTICERAL project: shape memory alloy films Ni2MnGa on ferroelectric layers and active substrates and also ferrites/ferroelectric composites.
- First-principles calculation (DFT) of structural, electronic and hyperfine properties of materials (oxides). At this stage, mainly application to manganite oxides.

b) High Temperature superconductors
-Physical characterization studies of oxide superconductor materials prepared by LFZ (BSCCO fibers: magnetic properties studies for critical current and superconducting fraction).
-MgB2-type superconductors: preparation and processing of Superconducting thin films on Si and sapphire substrates. Study of epitaxy and microstructure. Magnetic and electrical properties studies.

c) Magnetic Semiconductors.
-Magnetization and susceptibility studies on semiconductor films and low-dimensional structures: Patterned Fe silicides thin film structures with competition of magnetic anisotropy effects from shape and crystal orientation.

d) Theoretical study of magnetic systems and phase transitions.
-Magneto-electro-elastic coupling mechanisms. Development of mean-field approaches for data analysis and modeling. Application of original method (APL 2007) to analyse and separate contributions to the magnetic properties of ferromagnetic systems. Also applied to Fe nanoparticles in FeCu ball-milled alloys
-Development of fundamentals of Tsallis non-extensive statistics and applications to strongly correlated electron systems and other complex inhomogeneous magnetic systems. Theoretical analysis of NMR tomography to measure (non-extensive) systems out of equilibrium; i.e., excitation of two ½-spin nucleus to build a non-equilibrium density matrix; from this result it is possible to obtain all desired thermal properties, such as specific heat, magnetization and other quantities.
-Development of crystal field theory to understand the magnetic behavior of intermetalic compound, namely $Pr(Ni,Co)_5$.

Magnetocaloric Effect and Its Applications: Theory, Experiments and Prototype

a) Optimization of intermetallic/metalloid compounds for magnetocaloric applications
-Systems under study are mainly containing rare-earths and transition metals to provide magneto-structural coupling: Ni2MnGa, $Pr(Co,Ni)_5$, LaFeSi, MnBi and also manganites.
-Influence of interstitial hydrogen and nitrogen on the magnetocaloric properties of metals. Study of new preparations routes, such as ball milling (LaFeSi).

b) Modeling of magnetic entropy contributions for the understanding of material properties.
-This topic is developed in connection with item 2.4, focusing on magnetic entropy. Examples: mapping the magnetic stability among different phases (in first and second-order phase transitions), with magnetostructural effects.

c) Development of a new process to optimize thermo-magnetic cycles, in the sense of the magnetocaloric effect.

d) Modelling of components and building of a prototype for magnetocaloric refrigeration near room temperature. Development of pilot experiments on dynamic magnetocaloric effect.

Scientific Instrumentation

a) Upgrading of RF sputtering materials deposition system
-Design of a control system for co-deposition and multilayer deposition enabling automatic sequential control of power sources of targets and shutters

b) *Experimental set-up for electric measurements, with thermal-magneto expansion and magneto-resistance, from 77 K up to 500 K and from -1 Tesla up to 1 Tesla (rotating field, from 0º to 360º).*
Concluding the automation of the measurements.

c) Development of new experimental techniques up to 10 Tesla and temperature 1.6 K-300K in the VSM magnetometer cryostat/magnet
-New adjustments in the VSM probe
-Use of a Cu-Be pressure cell (up to 10 kBar)
-Electrical resistivity and magnetoresistance measurements with already available measurement cell requiring measurement adaptation and performance tests for optimization and automation
-Design of specific heat and thermal-magneto-expansion techniques.

REACTIVE CERAMIC COMPONENTS FOR PROCESS CONTROL

Materials For High-Temperature Electrochemical Applications. $Yb_2Ti_2O_7$-based materials will be used as model systems for quenched point defect chemistry developed on cooling from sintering temperatures, and by structural changes induced by anti-site cation distribution. Some additional work on apatite type solid electrolytes (including mechano-synthesis or mechanical activation) will be dedicated to improve the sinterability and to minimize formation of undue secondary phases

Deviations in potentiometric sensor readings are being re-examined to analyse the role of residual electronic transport number, factors determining the reversibility of electrode kinetics and geometric factors. Different solid electrolytes (e.g. YSZ, lanthanum gallate, cerias, etc.) will be used in these studies. Alternative methods are also been used to evaluate the mixed transport properties of ionic and mixed conductors, to emphasize differences between these methods and to design efficient modifications with minimized errors.

One will continue previous studies of correlations between the kinetics of oxygen reduction at CGO/cathode interfaces and the residual p-type electronic conductivity of the solid electrolyte. This minor p-type contribution can be adjusted by inducing bulk electronic conductivity by composition changes or preferential changes at grain boundaries, including changes in firing schedule or grain boundary additives.

Alternative electrode materials will be studied with an emphasis on potential electrodes for apatite-type solid electrolytes, with emphasis on generic systems $Sr_{1-x}Ce_xMn_{1-y}Cr_yO_{3-\delta}$ and $La_{1-x}Sr_xMn_{1-y}Ti_yO_{3-\delta}$. These studies will comprise total conductivity, Seebeck coefficient, thermal and chemical expansion, steady-state oxygen permeability in wide ranges of oxygen partial pressure range and temperature, and also stability ranges and oxygen stoichiometry changes. In addition, one will study the reactivity and/or interdiffusion with promising $La_{10}Si_{6-x}Al_xO_{26.5}$ or related apatite type electrolytes, and will assess the electrochemical performance of selected electrode compositions

The complex correlations between structural changes in $YBaCo_2O_{5.50}$ and its mixed transport properties are being revised based on structural refinement of diffraction data and magnetic properties. Similar studies will be started for other $LnBaCo_2O_{5+\delta}$ cobaltites with alternative lanthanides (e.g. Ln=Nd). These materials have proven high electrochemical performance and thus potential use as oxygen electrodes

Glass-ceramics compositions with high content of pyroxene phases, which are capable for wide isomorphous substitutions in their crystal structure and possess suitable physical and chemical characteristics will be studied as potential glass-ceramic seals. The aim is to investigate crystallization kinetics, the microstructure and other properties of glass-ceramics. We will assess the crystallization behavior of the diopside based glasses, microstructure changes and the properties of the sintered glass-ceramics, including its interaction and adhesion to 8YSZ and typical high temperature alloys.

Mixed Conducting Materials and Catalysts for Oxygen Separation or Partial Oxidation of Hydrocarbons. Developments on mixed conducting membranes will include a re-examination of correlations between composition changes, point defect chemistry (including defect interactions) and mixed transport properties of $La_2(Ni,Cu,Fe)O_{4+\delta}$ nickelates. Further modifications of dense $La_2NiO_{4+\delta}$ membranes will be focused on their catalytic activity, including ultrasonic treatments in liquid media, to enlarge the surface area, and deposition of $YBa_2Cu_3O_{7-\delta}$ thin films onto the feed-side surface. One will also continue studies of stability limits and redox behaviour under very reducing conditions, to assess the ability to redox tune catalytic properties promoted by the onset of reduced species.

Dense $(SrFeO_{3-\delta})_{1-x}(SrAl_2O_4)_x$ (SFSA) composite membranes prepared in tubular form will be assessed under prospective worling conditions, i.e., air/inert atmpsphere and air/CH_4 gradients, and tested as model systems for partial oxidation of methane, including their transport properties, selectivity, catalytic efficiency, chemical and thermomechanical stability and CO_2 tolerance. Further work will also be performed to optimize the processing of 2-layer porous-dense mixed conducting membranes and studying its impact on oxygen permeability. A reference system comprising a porous $La_{0.5}Sr_{0.5}FeO_{3-\delta}$ layer and a dense layer of $SrFeO_{3-\delta}$-$(SrAl_2O_4)$ composites will be appraised, including improvements in processing of pore-dense membranes, and assessment of their oxygen permeation properties and selectivity for partial oxidation of methane.

Microstructural Effects. Further prospects of grain boundary engineering will be explored based on heterogeneous ceramics, as expected for materials with designed core-shell structures or less common possibilities of designing ceramics with ionic conducting grain interiors and electronic conducting grain boundaries. Some of these attempts will be based on selective (and fast) grain boundary diffusion. Other attempts will be focused on circumventing the limitations of blocking grain boundaries, as for ceria-based materials contaminated with silica.
Ceria-based solid electrolytes are been used as model systems to examine the role of impurities on grain boundary transport properties and to design strategies to minimize those effects. The two main approaches are based on sintering additives to lower the firing temperatures and thus the risk of high temperature contaminations, and microstructural changes to promote concentration of impurities in isolated impurity containing phases, or even formation of new silicate-type ion conductors, such as apatites.

Materials for Other Electrochemical Technologies. Different phases in the systems Ca-Fe-O (e.g. $CaFe_2O_{4-\delta}$ and $Ca_2Fe_2O_{5-\delta}$) are being studied as potential mixed conductors for high temperature electrochemical application. The transport properties will be measured and analysed to determine the main factors affecting the electronic and ionic conductivities, and as guidelines for optimization. This will include the possibility of cation redistributions and redox behaviour of some of these materials. Stability limits will be revised to establish applicability ranges.
One will also continue studies of oxygen electrodes for electrolytic in aqueous media, by extending the range of working conditions, such as temperatures approaching boiling conditions, higher alkalinity in aqueous solutions, use of suspensions, stirring, etc., to obtain guidelines to improve the electrode materials and optimize operation conditions in terms of electrocatalytic activity, degradation and prospective electrode regeneration.

Diamond Coatings. Multilayer coatings of CVD microcrystalline and nanocrystalline diamond (MCD/NCD) coatings will combine both the superior adhesion of MCD and the surface properties of NCD in a multilayered composite coating. Alternate MCD/NCD thin layers will prevent MCD grains to grow excessively allowing a smooth surface by depositing a top NCD layer, while enhanced fracture toughness is achieved by careful interlayer design.
The machining of abrasive materials such as sintered ceramics, graphite and aluminium alloys by CVD diamond coated tools will be further developed. Other materials such as ultra-fine or nano-sized hardmetals will be diamond coated after careful selection of the surface treatments needed to enhance the adhesion of CVD diamond coatings.

Other Hard and Ultra-Hard Materials. Innovative processing of ceramics using laser technology will be a new research subject, namely the design of microstructures capable of withstanding high to ultrahigh temperatures and the laser assisted machining of ceramic materials.
The activities of the research group include foundation of a spin-off company with industry support, and several other projects to strengthen relationships with industry.

Processing Methods. Colloidal processing of SiAlON based materials reinforced with rod-like α-SiAlON particles will be developed aiming to obtain high strength and hardness, good wear resistance, and thermal shock resistent ceramics. Different densification methods will be used, including pressureless sintering, hot pressing, HIPing and spark plasma sintering. Sintering conditions will be correlated to machanical and tribological properties. Other composite materials based on Al_2O_3, $MgAl_2O_4$ spinel, ZrO_2–$MgAl_2O_4$ and Al_2O_3-ZrO_2 will be also processed and characterized for their relevant properties. Continuation will be given to previous work on the colloidal processing and sintering of SiC ceramics.

Corrosion Protection Methods. The research activity planed for 2008 will be focused on the main directions started in recent years. The main research topics will be on development of new active corrosion protection systems for different metallic substrates. Investigations will be concentrated on the idea of developing active corrosion protective coatings with self-healing ability in frame of several scientific projects.
The new nanocontainers of corrosion inhibitors will be developed to be used as anticorrosive pigments in different protective coatings. Other active agents such as water repellents will also be nanoencapsulated in order to provide multi-level active protection systems.
Studies of mechanism of corrosion processes and corrosion inhibition will be continued in 2007. New organic and inorganic corrosion inhibitors will be tested for the different steel, aluminum alloy and magnesium alloy substrates.
The Scanning Vibrating Electrode Technique (SVET) and Scanning Ion-selective Electrode Technique (SIET) will be employed to get fundamental understanding of the localized corrosion processes in the micro-confined defects in organic coatings on metallic substrates. The SVET/SIET method itself will be in focus of planned research. The applicability of these techniques to study self-healing properties of protective will be tested. The new ion-selective electrodes for measurement of active species in the electrolyte near the active metal surface will be developed and applied.
Novel anodic oxide films produced by the powerful electric discharge method on titanium will be studied from standpoint of their semiconductive and protective properties.

WASTES RECYCLING AND GREEN PRODUCTS

Different types of recycling industrial wastes and by-products will be characterized and incorporated in new materials with potential added-values. Current research will be extended to other types of residues in order to find suitable solutions for cleaner environment, to preserve natural and non-renewable resources or save energy, while improving some of the actually existing products or developing new ones with new functionalities.
The historic and architectonic value of adobe built heritage must be preserved, not only by the uniqueness of its construction but also due to the identity and memory that it represents and the sustainable development involved. Work is under development in order to constitute a knowledge matrix that guides the development of compatible mortars for heritage preservation.
Study of the formation and behaviour of sustainable construction materials involving mortars and wastes has started. Research on the setting mechanism of several formulations with wastes from a biomass plant (fly ashes) in a cement matrix is being performed in terms of hydration contribution and other features.

MACROMOLECULAR MATERIALS AND BIOREFINERIES

Novel Biomass-Derived Materials and Composites. Within the scope of the development of new cellulose-based materials, future work will be focused mainly on the investigation of new strategies for the controlled heterogenous modification of cellulose substrates, in particular bacterial cellulose, and on the potential applications of the new cellulose derivatives already obtained. The development of new cellulose-based composites will be reinforced. The research on the development of new materials based on starch will be continued.
Among the chitosan based materials which are going to be investigated, different blends and coatings will receive much attention, together with the elaboration of reversible hydrogels based on the application of the Diels-Alder reaction to appropriately modified chitosan macromolecules.
In the context of furanic polymers, the coming year will be mainly devoted to the synthesis of polymeric materials starting from the monomers prepared so far, to the study of the reversibility of the Diels-Alder polymerization (using NMR, viscosity and UV techniques) and to the detailed characterization of the ensuing materials.
Research on new cellulose/inorganic particles nanocomposite materials and its incorporation on polymer matrix based composites will be pursued.
A prototype for evaluating the thermal behaviour of lignocellulosics-based phase change materials composites, at present under study, will be ready for tests during next year. The evaluation of new compounds to be used as phase-change materials will continue. The studies with fatty acids will be completed and attention will be now devoted mainly to the fatty acid esters as phase change materials as they could be easily recovered from the biodiesel production at much lower costs than paraffins. Attention will also be paid to other hydrocarbons, such as the alkylbenzenes.

Upgrading Cork and Wood Pulping by-Products. The development of new polyesters based on suberin components will reach a partial conclusion, with the end of the European project within which it is being developed.
Two research projects related to the utilization of by-products from the acid sulphite pulping of *E. globulus* wood (condensates from pulping liquor evaporation and the components of sulphite spent liquor) will be accomplished next year.

Wood Pulping and Bleaching. The work on highly selective polyoxometalate (POM) catalysis in oxygen delignification of kraft pulp using POMs will be continued. The application of a new electronic tongue (ET) multisensor system for the detection of particular structures of polyoxometalates containing vanadium (IV/V) atoms and for the monitoring of their behaviour in redox catalysis will be continued.
The study on the paper surface modification with perspective formulations prepared using sol-gel process will continue. The main efforts will be done on the pilot trial on the deposition of nanoformulations on the paper surface and the evaluation of coated paper response for the ink-jet and off-set printing quality. The new functional cellulose-silica hybrid materials will be synthesised, characterised and tested in the redox catalysis.

Structural Studies of Lignocellulosic Materials. The studies on ESI-MS application for the structural characterization of lignins will continue. The studies on specific structural features of hardwood hemicelluloses employing ESI-MS/MS and MALDI-TOF/TOF will be pursued. The study on the chemical composition of macromolecular components of the natural hybrid of *Paulownia elongata* and *Paulownia fortunei* will be further developed. The study on the chemical and structural characterization of grape skins and stalks will be continuing. The role of several depolymerising enzymes and fungi on the detailed nanostructure of cork will be continued, with strong emphasis on the direct characterisation of the complex material by NMR and FTIR methods.

Chemical Conversion of Biomass Into Chemicals. We will continue to investigate routes for the chemical valorisation of carbohydrates, namely acid-catalysed dehydration of ketoses into furan derivatives using porous heterogeneous catalysts and base-catalysed isomerization of ketoses into added value products, such as transformation of glucose into fructose, using porous solid bases.

Other Polymer Systems and Polymer-Based Nanocomposites. Work demonstrating the existence of local ordered regions in polymer melts will be finished. Works dealing with the effect of shear-pulses on the melt morphology of ionomers, slightly crossllinked polymers and polymers synthesized from different catalysts, already finished, will also terminate.
A new time-lag apparatus for the measurement of gas and vapours permeability that we have been building will be ready. Barrier properties for the developed materials will be measured and according to these results modified polymeric materials for active packaging will be developed. The field of active transport in polymeric materials will be further explored for other applications, namely olefin/paraffin separation.
Studies on aqueous based polymerisation systems (namely microemulsion and miniemulsion) for the preparation of NCs materials via living polymerisation will receive particular attention.
As regards the polysaccharide NC project, exopolysaccharides produced by *Rhyzobium sp* will be tested as well as the preparation of thin films from such composites.
The conducting properties of the NCs prepared will be investigated. Modified carbon nanotubes and CNFs polymer based NCs will be investigated. Focus will be given to the influence of interface on the resulting mechanical properties.

Biofuels. We will address the purification of biodiesel in the current production process. We are particularly interested in the removal of glycerol, fatty acids, and catalyst from the biodiesel by extraction with water in counter current. Measurements of solubility of fatty acids and fatty acid esters in water and water in the biodiesel current will be carried. The modelling of the systems will be attempted using the CPA-EoS model. These results will also allow the prediction of the water solubility in the Bx mixtures from the knowledge of the fuel composition. Another important issue to be addressed will be the low temperature behaviour of the Bx mixtures. Cloud points will be measured for biodiesels and Bx mixtures and their values will be modelled using the Predictive UNIQUAC.
The production of lipase will continue being an issue of research during this year. Characteristics of the PFCs not yet fully explored will continue being studied and the mass transfer coefficients and their impact on the lipase production will be evaluated.
Two phase aqueous systems and the extraction of lipase using ioinic liquids will also be a major subject of research during this year. The characterization of various properties of the ionic liquids relevant for their design and use will be addressed.
Reseaarch on the flash pyrolysis of *E. globulus* wood (liquefication) will be initiated.

BIOMEDICAL AND BIOMIMETIC MATERIALS

Biomaterials and Biological Systems. Special attention will be given to the processing parameters of the developed formulations and specimens in order to control and optimize their production in a reproducible way.
In vitro tests in accellular and in cellular media will proceed with selected materials to assess their inorganic and biological reactivity.
Scaffolds of adequate porosity and mechanical properties and a number of composites will be loaded with therapeutic agents to study drug leaching rate of various medicals.
In vivo tests and histological studies in mouse kidney, spleen and liver will continue with other selected materials to assess their biocompatibility.
Chemically derivatised newly developed biomaterials based on magnetic nanoparticles (magnetite/carrageenan) will be functionalised for antibody specific recognition of cancer cells and their efficiency tested in vitro. The controlled release of magnetic particles will be characterised and monitored.
The NMR characterisation of biofluids and biological tissues will been pursued for application in the following areas: (i) study of pregnancy disorders, (ii) heart failure and diabetes incidence, (iii) detection of inborn errors in newborn babies and d) biological tissues analysis for cancer diagnosis.
The metabonomic study of ostheocarsome cells will be pursued by HR-MAS NMR, in order to establish the normal metabolic profiles of these cancer cells and then go on to study the effects of several new drugs under chemical development.
The search for suitable conditions for the growth of mHBP and mHBP-PPIX crystals will be carried out. Heavy atom replacement for x-ray structure determination of hSOUL, via production of SeMet-hSOUL, will be continued. High field NMR data for hSOUL will be analysed. Molecular modelling of the mHBP-PPIX and mHBP-hemin systems will be continued and extended to include the hSOUL system.
NMR/LC-NMR analysis for amniotic fluid, urine and blood samples from pregnant women will be continued and extended to include mass spec data. As more samples are analysed PCA will be carried out and extended to include PLS-DA for disease characterisation.

***Structural Studies of Porphyrins and Corroles*.** The elucidation of the structural details of [60]fulleropyrrolidine-nucleoside conjugates, prepared from formylpyrimidone derivatives, *N*-methylglycine and C_{60} via 1,3-dipolar cycloaddition reactions, will be attempted.

Artificial Receptors for Pharmaceutical and Environmental Applications. With a view to mimicking and understanding molecular recognition processes in biological systems, research for the next year will be focussed on the development of artificial receptors for the selective binding and sensing of the substrates with biological relevance and medicinal application. This work will be carried out using experimental and theoretical methods. A particular attention will be dedicated to the following specific topics:
Development of novel aza-bridged calixarene receptors based on calix[2]arene[2]triazine architectures for medicinal chemistry application:
This project is concerned with the molecular design and synthesis of artificial receptors composed of two phenyl rings and two triazine rings linked by nitrogen bridges. Subsequently these receptors will be used on the binding studies with chiral drugs from the families of barbiturates, 1,4-dydropyridines and nucleoside derivatives.

The binding interaction between the azacalix[2]arene[2]triazine derivatives and the chiral drugs will be investigated in solution by NMR methods and in solid state by single crystal X-ray diffraction. The receptors with higher binding affinities for the chiral substrates will be immobilised onto silica gel affording chiral stationary phases and their enantioselective resolution capabilities will be evaluated in HPLC columns using directly marketed racemic drugs. The molecular modelling studies will be used extensively as a complementing and a supportive tool to enhance our understanding the binding interaction between the receptors and the substrates.

- Molecular design of artificial receptors for anion and ion pair recognition:

This project is concerned with molecular design of receptors for the molecular recognition of anions and ion pairs with biological relevance via simulation tools. The receptors include molecular machines, rotaxanes and catenanes, as well as heteroditopic receptors with inophore properties.

- Computational studies of the diffusion of delivery-systems in cellular membranes models:

This project aims the application of computational simulation tools to the study of the molecular recognition mechanisms between synthetic receptors and substrates with pharmacological interest. Furthermore, the interaction and diffusion of these host-guest systems with model membranes will also be addressed. The modelling work includes the following tasks:

a) Study of the host-guest interaction, docking and calculation of binding constants;

b) Extensive understanding of the host interaction with a model membrane: diffusion, free energy profiles;

c) Investigation of the diffusion mechanisms of the supramolecular host-guest systems through the model membranes. The artificial receptors comprise dendrimers and calixarene based architectures.

At the long term this project aims the *in silico* design of new transporters with enhanced diffusion capacities through the cellular membranes and which are capable to act as drug-delivery systems.

- Molecular recognition mechanisms of tetrapyrroles by heme binding proteins:

The main goal of this project is the understanding of the structure and function of heme binding proteins (HBP), such as the human and rat p22HBP protein, by means of computational simulation methods. The ligands comprise the heme b and anabolic and catabolic molecular intermediates such as protoporphyrin IX and bilirubin. This line of research will focus on the protein binding properties of the heme and it will have implications in the fundamental understanding of the tight cellular regulation and homoeostasis of the heme and iron, and will address biomedical concerns of heme related diseases such as porphyrias. We will address the following research sub-topics: (i) Parameterization of tetrapyrroles involved in the catabolism and anabolism of the heme using quantum mechanics calculations. (ii) Docking studies between the heme and derived tetrapyrroles and HBPs in order to find out the molecular recognition models for subsequent simulations studies. (iii) Extensive molecular dynamics and free energy studies of binding of the HBPs free in solution and in complex with the heme and tetrapyrroles. (iv) Understanding the molecular implications of several HBPs point mutations reported in the literature on protein function by *in silico* simulations of the protein mutations.

Metal Complexes of Bio-Inorganic Interest. New chromium compounds taken as models for relevant intermediates in the intracellular-Cr(VI) reduction will continue to be studied by several techniques (including EPR). Additionally some chromium nutritional important compounds will be synthesised and tested (*in vivo*), as they have become suspicious to provoke damages *in vivo*.

Mass spectrometry studies with Ru(II) complexes: binuclear Ru(II)-thioether systems are intended to continue to be elucidated by ESI-MS and ESI-MS/MS, in order to establish fragmentation patterns and mechanisms. Ru(II)-aminoacids new compounds, particularly useful to mimic interactions with proteins and DNA constituents, will also be explored.

SECTION 4
Scientific Production

PhD Theses

CARACTERIZAÇÃO DE NOVOS MATERIAIS DE EMBALAGEM COM ÊNFASE EM POLÍMEROS BIODEGRADÁVEIS
PEDROSA NM
COUTINHO JAP; MARRUCHO IM
UNIVERSITY OF AVEIRO, 2007

CARDOSINA A COMO MODELO PARA O ESTUDO DA ESTABILIDADE CONFORMACIONAL DE PROTEINASES ASPÁRTICAS
PEREIRA AO
BARROS M; PEREIRA ML
UNIVERSITY OF AVEIRO, 2007

CONVERSÃO DE XILANAS A FURFURAL NA PRESENÇA DE SÓLIDOS ÁCIDOS MESOPOROSOS
DIAS ASVS
VALENTE AA; PILLINGER M
UNIVERSITY OF AVEIRO, 2007

DIAMANTE CVD NANO- E MICROCRISTALINO PARA CORTE DE MATERIAIS ABRASIVOS
ALMEIDA FA
SILVA RF
UNIVERSITY OF AVEIRO, 2007

ELECTRÓLITOS SÓLIDOS PARA SENSORES ELECTROQUÍMICOS
LIMA EMCLGP
MARQUES FMB; FIGUEIREDO FMHLR
UNIVERSITY OF AVEIRO, 2007

ESTUDO DA COMPOSIÇÃO E VALORIZAÇÃO QUÍMICA DE DIFERENTES PARTES MORFOLÓGICAS DA BANANEIRA *"DWARF CAVENDISH"*
OLIVEIRA L
SILVESTRE AJD; CORDEIRO NA
UNIVERSITY OF AVEIRO, 2007

LIGAÇÕES DE HIDROGÉNIO C-H•••O EM ESTRUTURAS SUPRAMOLECULARES
NOLASCO MM
RIBEIRO-CLARO PJA
UNIVERSITY OF AVEIRO, 2007

NMR STUDIES OF MURINE ALAS AND MURINE P22HBP: TWO PROTEINS INVOLVED IN HEME METABOLISM
DIAS JS
GOODFELLOW BJ; MACEDO AL
UNIVERSITY NOVA OF LISBON, 2007

PARTIAL OXYOROPYLATION OF POLYSACCHARIDES: SYNTHESIS OF NOVEL COMPOSITE MATERIALS
MENEZES J
GANDINI A
UNIVERSITY OF SÃO PAULO, BRAZIL, 2007

PREPARATION AND PROPERTIES OF $SRBI_2M_2O_9$ (M= TA, NB) THIN FILMS
AGUILAR G G
COSTA MEV; SALVADO IMM
UNIVERSITY OF AVEIRO, 2007

PRODUÇÃO DE LIPASE POR *YARROWIA LIPOLYTICA* EM BIORREATOR MULTIFÁSICO
AMARAL PFF
COUTINHO JAP; COELHO MAZ
UFRJ 2007

REDES HIBRIDAS ORGÂNICAS/INORGÂNICAS INCORPORADAS COM COMPLEXOS DE ÍONS LANTANIDEOS
LIMA P P
MALTA OL; CARLOS LD
FEDERAL UNIVERSITY OF PERNAMBUCO, BRASIL, 2007

REVESTIMENTOS DE DIAMANTE NANOCRISTALINO PARA APLICAÇÕES BIOMÉDICAS
AMARAL M S
SILVA RF; SANTOS JD
UNIVERSITY OF AVEIRO, 2007

SOLUBILIDADE E TRANSFERÊNCIA DE MASSA EM SISTEMAS ORGÂNICOS DISPERSOS EM FASE AQUOSA
MARTINS MGF
COUTINHO JAP; MARRUCHO IM
UNIVERSITY OF AVEIRO, 2007

SYNTHESIS AND CHARACTERISATION OF NEW LAYERED AND MICROPOROUS PHOTOLUMINESCENCT SILICATES
KOSTOVA M H
ROCHA J; CARLOS LD
UNIVERSITY OF AVEIRO, 2007

SYNTHESIS AND CHARACTERIZATION OF POLYMER MATRIX FUNCTIONAL NANOCOMPOSITES
ESTEVES A C C
BARROS-TIMMONS A; TRINDADE T
UNIVERSITY OF AVEIRO, 2007

A ESCOLA NA PREVENÇÃO DE COMPORTAMENTOS DE RISCO: O TABAGISMO E O CONSUMO DE ÁLCOOL
CASAL AA
PEREIRA ML; BATISTA L
UNIVERSITY OF AVEIRO, 2007

APLICAÇÃO DE MÉTODOS AB INICIO AO CÁLCULO DE PARÂMETROS HIPERFINOS EM ÓXIDOS MAGNÉTICOS
GONÇALVES JNS
AMARAL VS
MSC PHYSICAL ENGINEERING, UNIVERSITY OF AVEIRO 2007

APLICAÇÕES DO EFEITO MAGNETOCALÓRICO: DESIGN EAUTOMATIZAÇÃO DE DISPOSITIVOS
FERNANDES NAD
REIS MS; AMARAL VS
MSC PHYSICAL ENGINEERING, UNIVERSITY OF AVEIRO 2007

AVALIAÇÃO DO EFEITO DO CHUMBO NA QUALIDADE ESPERMÁTICA DE HUMANOS E DE RATINHOS
SILVA TA
PEREIRA ML; ALMEIDA V
UNIVERSITY OF AVEIRO 2007

BORON NITRIDE THIN FILMS DEPOSITED BY MAGNETRON SPUTTERING ON SI_3N_4
CONCEIÇÃO JC
SILVA RF
UNIVERSITY OF AVEIRO 2007

CARACTERIZAÇÃO POR CROMATOGRAFIA GASOSA DE ÓLEOS VEGETAIS E CERAS PARAFÍNICAS
MIRANTE FIC
COUTINHO JAP; SILVESTRE AJ
UNIVERSITY OF AVEIRO 2007

CINÉTICA DE FORMAÇÃO DE ALDEÍDO SIRÍNGICO DURANTE A OXIDAÇÃO DE LENHOSSULFONATOS COM OXIGÉNIO EM MEIO ALKALINO
SANTOS SGM
EVTYUGIN DV
UNIVERSITY OF AVEIRO 2007

CONTRIBUTOS PARA UMA OBSERVAÇÃO EFECTIVA DO DESIGN EM PORTUGAL
LIMA PG
SILVA RF; BRANCO JS
UNIVERSITY OF AVEIRO 2007

CONCEPÇÕES E PRÁTICAS CTS DOS PROFESSORES DE UMA ESCOLA INOVADORA
TRÉZ TA
PEDROSA J, VIEIRA R
UNIVERSIDADE DE AVEIRO, 2007

DESLENHIFICAÇÃO ELECTROQUÍMICA DE PASTA KRAFT USANDO POLIOXOMETALATO COMO INTERMEDIÁRIO
MARTINS MRRC
EVTYUGIN DV
UNIVERSITY OF AVEIRO 2007

EFFECT OF CARBON NANOFIBRES FUNCTIONALISATION ON THERMAL AND MECHANICAL PROPERTIES OF PA12/CNF NANOCOMPOSITES
GHISLANDI M
BARROS TIMMONS AMV; SCHULTE K
(EMMS) UNIVERSITY OF AVEIRO | TECHNISCHE UNIVERSITÄT
HAMBURG-HARBURG 2007

ENERGIAS RENOVÁVEIS EM PORTUGAL - SITUAÇÃO ACTUAL. CONTRIBUTOS PARA A SUA DIVULGAÇÃO
LOPES BS
MAGALHÃES MCF
UNIVERSITY OF AVEIRO 2007

EQUILÍBRIO LÍQUIDO-LÍQUIDO NA PRODUÇÃO DE BIODIESEL
CARVALHO SAES
COUTINHO JAP; MARRUCHO IM
UNIVERSITY OF AVEIRO 2007

ESTUDO DE SUPERCONDUTORES CERÂMICOS: MGB_2
PINHO RJCA
AMARAL VS; COSTA F
MSC APPLIED PHYSICS, UNIVERSITY OF AVEIRO 2007

EVALUATION OF COSMO-RS FOR HENRY CONSTANTS AND SELECTIVITY PREDICTION
FILIPE LMB
COUTINHO JAP; MARRUCHO IM
UNIVERSITY OF AVEIRO 2007

EXPRESSÃO DE PROTEÍNAS DAS VIAS DE APOPTOSE NAS CÉLULAS ESTAMINAIS E PROGENITORAS DO EPITÉLIO GERMINAL MASCULINO
RICARDO AL
SOUSA M; PEREIRA ML
UNIVERSITY OF AVEIRO 2007

FABRICATION OF ORGANIC FIELD-EFFECT TRANSISTORS AND AB INITIO INVESTIGATION OF THE ELECTRONIC TRANSPORT PROPERTIES OF STIRRED AND NON-STIRRED POLYANILINE, SIO_2-POLYANILINE, AND $SIO_2@FE_2O_3$-POLYANILINE
CHIMAMKPAM EFC
BARROS TIMMONS AMV; BAUHOFER W
(EMMS) UNIVERSITY OF AVEIRO | TECHNISCHE UNIVERSITÄT
HAMBURG-HARBURG 2007

FILMES DE DLC PARA APLICAÇÕES BIOTRIBOLÓGICAS
SALGUEIREDO E
SILVA RF; COSTA FM
UNIVERSITY OF AVEIRO 2007

GEOPOLIMERIZAÇÃO DE DIFERENTES MISTURAS DE RESÍDUOS INDUSTRIAIS
MENDONÇA C
LABRINCHA JA; FERREIRA VM
UNIVERSITY OF AVEIRO 2007

HISTÓRIA DO DESIGN DE VEÍCULOS AUTOMÓVEIS EM PORTUGAL
RUFO EC
SILVA RF; AGUIAR C
UNIVERSITY OF AVEIRO 2007

INVESTIGATION OF FERROELECTRIC DOMAINS WITH SCANNING PROBE MICROSCOPY
FERNANDES RP
SCHNEIDER G; AMARAL VS; REIS MS
(EMMS) UNIVERSITY OF AVEIRO | TECHNISCHE UNIVERSITÄT HAMBURG-HARBURG 2007

MEDIÇÃO DE EQUILÍBRIOS GÁS LÍQUIDO A ALTAS PRESSÕES
VENTURA SPM
COUTINHO JAP; MARRUCHO IM
UNIVERSITY OF AVEIRO 2007

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MAFRA L; ROCHA J
TARRAGONA, SPAIN, 01-06 JUL 2007, 2^{ND} IBEROAMERICAN NMR MEETING

HYPERFINE STUDIES ON MULTIFERROIC $RMnO_3$ COMPOUNDS
AMARAL JS; MENDONÇA TM; PEREIRA AM; FIGUEIRAS F; REIS MS; LOPES AML; ARAÚJO JP; AMARAL VS; CORREIA JG; TAVARES PB
PORTO, PORTUGAL, 2007, 31^{ST} INTERNATIONAL SYMPOSIUM ON DYNAMICAL PROPERTIES OF SOLIDS (DYPROSO XXXI)

INTERPRETING AND MODELING MAGNETOCALORIC DATA AND PROPERTIES: THE LANDAU THEORY OF PHASE TRANSITIONS AND MEAN-FIELD THEORY
AMARAL JS; AMARAL VS
PORTOROZ, SLOVENIA, 2007, SECOND INTERNATIONAL CONFERENCE OF THE INTERNATIONAL INSTITUTE OF REFRIGERATION IIF/IIR ON MAGNETIC REFRIGERATION AT ROOM TEMPERATURE

JAHN-TELLER POLARON CLUSTERS IN FERROMAGNETIC INSULATOR MANGANITES
LOPES ML; ARAÚJO JP; RAMASCO JJ; AMARAL, VS; SURYANARAYANAN R; CORREIA JG
PORTO, PORTUGAL, 2007, 31^{ST} INTERNATIONAL SYMPOSIUM ON DYNAMICAL PROPERTIES OF SOLIDS (DYPROSO XXXI)

LOCAL PROBE EVIDENCES FOR ELECTRICAL POLARIZATION IN CHARGE ORDERED $PR_{1-X}CA_XMNO_3$ MANGANITES
LOPES AML; ARAÚJO JP; AMARAL VS; CORREIA JG; TOMIOKA Y; TOKURA Y
PORTO, PORTUGAL, 2007, 31^{ST} INTERNATIONAL SYMPOSIUM ON DYNAMICAL PROPERTIES OF SOLIDS (DYPROSO XXXI)

LOCAL PROBE STUDIES ON HIGHLY DISTORTED RARE-EARTH MANGANITES
MENDONÇA TM; AMARAL JS; PEREIRA AM; FIGUEIRAS F; REIS MS; LOPES AML; ARAÚJO JP; AMARAL VS; CORREIA JG; TAVARES PB
GENEVA, SWITZERLAND, DEC 2007, ISOLDE WORKSHOP AND USER'S MEETING, CERN

LOCAL PROBING OF ELECTRIC AND MAGNETIC ORDER COEXISTENCE IN MANGANITE SYSTEMS
LOPES AML; ARAÚJO JP; CORREIA JG; AMARAL VS; MENDONÇA TM; REIS MS; TAVARES PB; FIGUEIRAS F; AMARAL JS; PEREIRA A; SILVA MR; TOMIOKA Y; TOKURA Y AND THE ISOLDE COLABORATION
GENEVA, SWITZERLAND, DEC 2007, ISOLDE WORKSHOP AND USER'S MEETING, CERN

MAGNETORESISTIVE MATERIALS: HYPERFINE STUDIES USING RADIOACTIVE ISOTOPES
AMARAL VS; CORREIA JG; ARAÚJO JP; LOPES AML; TAVARES PB; MENDONÇA TM; AMARAL JS; GONÇALVES J
GENEVA, SWITZERLAND, DEC 2007, ISOLDE WORKSHOP AND USER'S MEETING, CERN

PHASE SEPARATION OF $La_{0.70-X}Er_XSr_{0.30}MnO_3$ AND ITS EFFECT ON MAGNETIC AND MAGNETOCALORIC PROPERTIES
AMARAL JS; REIS MS; ARAÚJO JP; MENDONÇA TM; TAVARES PB; AMARAL VS; VIEIRA JM
PORTO, PORTUGAL, 2007, IV INTERNATIONAL MATERIALS SYMPOSIUM AND XIII ENCONTRO DA SPM, MATERIAIS 2007

PRODUÇÃO DE OXIGÉNIO POR ADSORÇÃO COM MODULAÇÃO DE PRESSÃO
RAINHO JP, FRANCISCO A. DA SILVA F
2007, 7, NO ÂMBITO DO NOVO MESTRADO INTEGRADO EM ENGENHARIA QUÍMICA

RESOLUÇÃO DE ESTRUTURAS POR ESPECTROSCOPIA DE RMN DE SÓLIDOS
MAFRA L
COIMBRA, PORTUGAL, 07 DEC 2007, 1º SIMPÓSIO "RUMOS DA TECNOLOGIA FARMACEUTICA"

SHORT AND LONG RANGE ORDER IN SILICATES WITH Cu^{2+} CHAINS
MOREIRA DOS SANTOS A; AMARAL VS; BRANDAO P; ALMEIDA PAZ FA; ROCHA J; FERREIRA LP; GODINHO M; TRISTAN N; KLINGELER R; BÜCHNER B; DRECHSLER S; VOLKOVA O; VASILIEV A
TRIESTE, ITALY, 2007, WORKSHOP ON HIGHLY FRUSTRATED MAGNETISM

SÍNTESIS Y MODELIZACIÓN ESTRUTURAL DE UN HÍBRIDO ORGANO-INORGÁNICO, $TI(H_2PO_4)(PO_4)_{0.5}C_2H_5NH_2{}_{0.5}H_2O$, RELACIONADO CON EL -FOSFATO DE TITANIO
ESPINA A; KHAINAKOV SA; GARCÍA JR; GARCÍA-GRANDA S; MAFRA L ROCHA J; FERNÁNDEZ C
TOLEDO, SPAIN, 09-14 SEPT 2007, XXXI REUNION BIENAL DE LA RSEQ

SOLID-STATE NMR STUDIES OF POLYMORPHS IN DRUGS: METHODS AND APPLICATIONS
MAFRA L, LOURES
PORTUGAL, 26 JAN 2007, HOVIONE, LDA.

STRUCTURAL AND MAGNETIC STUDIES ON IRON OXIDE NANOPARTICLES IN HYBRID AND POLYMERIC MATRICES
SILVA NJO; CARLOS LD; AMARAL VS; DE ZEA BERMUDEZ V; MILLÁN A; URTIZBEREA A; PALACIO F
SEVILHA, SPAIN, 2007, NANOSPAIN

STRUCTURE AND PROPERTIES OF LANTHANIDE-ORGANIC POLYMERS WITH PICOLINIC AND GLUTARIC ACID
GIRGINOVA PI; PAZ FAA; PCR SOARES-SANTOS PCR; CARLOS LD; AMARAL VS; KLINOWSKI J; NOGUEIRA HIS; TRINDADE T
LONDON, UK, 02-05 JUL 2007, ADVANCING MATERIALS BY CHEMICAL DESIGN

STUDY OF LAYERED γ-TITANIUM PHOSPHATE INTERCALATED WITH N-ALKYLAMINES USING HIGH-RESOLUTION SOLID-STATE NMR, POWDER X-RAY DIFFRACTION AND MOLECULAR MODELING
MAFRA L; ESPINA A; KHAINAKOV SA; GARCÍA JR; ROCHA J; FERNANDEZ C
TARRAGONA, SPAIN, 01-06 JUL 2007, EUROMAR MAGNETIC RESONANCE CONFERENCE

SYNTHESIS AND FERRIMAGNETIC BEHAVIOUR OF MIXED METAL LEUCOPHOSPHITE
SHI F-N; DOS SANTOS AM; AMARAL VS; TRINDADE T; ROCHA J
STRASBOURG, FRANÇA, 2007, P1-17, EMRS 2007 SPRING MEETING, SYMPOSIUM R: DESIGN, CHARACTERISATION AND MODELLING OF MOLECULE-BASED, MAGNETIC MATERIALS

THE MAGNETOCALORIC EFFECT OF FERROMAGNETIC MANGANITES: MODELING AND INTERPRETATION OF PROPERTIES WITH LANDAU AND MEAN FIELD THEORY
AMARAL JS; REIS MS; ARAÚJO JP; MENDONÇA TM; TAVARES PB; AMARAL VS; VIEIRA JM
PORTO, PORTUGAL, 2007, 13^{TH} WORKSHOP ON MAGNETISM AND INTERMETALLICS

USING STATISTICAL DISTRIBUTIONS TO INVESTIGATE SIZE DEPENDENCE OF ANISOTROPY ENERGY AND MAGNETIC MOMENT IN ANTIFERROMAGNETIC FERRIHYDRITE NANOPARTICLES
SILVA NJO; AMARAL VS; CARLOS LD; RODRÍGUEZ-GONZÁLEZ B; LIZ-MARZÁN LM; BERQUÓ T; DE ZEA BERMUDEZ V; URTIZBEREA A; ARIZAGA A; MILLAN A; PALACIO F
ROMA, ITLAY, 2007, ICFPM: INTERNATIONAL CONFERENCE ON FINE PARTICLE MAGNETISM

VALORIZAÇÃO DE ESCÓRIAS DA INCINERAÇÃO DE RESÍDUOS SÓLIDOS URBANOS - PRODUÇÃO DE VIDROS E VITROCERÂMICOS
MONTEIRO RCC; FERNANDES MHV
PORTUGAL, 2007, 6, 39-41, VALORIZAÇÃO DE RESÍDUOS, CENTRO PARA A VALORIZAÇÃO DE RESÍDUOS

11TH EURO CONFERENCE ON THE SCIENCE AND TECHNOLOGY OF IONICS
MARQUES FMB (INTERNATIONAL SCIENTIFIC COMMITTEE)
BATZ-SUR-MER, FRANCE, 09-15 SEPT 2007

1ST SMARTER CRYSTALLOGRAPHY WORKSHOP
RIBEIRO-CLARO P, MAFRA L, ALMEIDA PAZ FA (ORGANIZING COMMITTEE)
AVEIRO, PORTUGAL, 06-07 SEPT 2007

30TH INTERNATIONAL CONFERENCE ON SOLUTION CHEMISTRY
MAGALHÃES MCF (SCIENTIFIC ADVISORY COMMITTEE)
MURDOCH UNIVERSITY, PERTH, AUSTRALIA, 16-20 JUL 2007

5º ENCONTRO NACIONAL DA DIVISÃO DE ENSINO E DIVULGAÇÃO DA QUÍMICA DA SOCIEDADE PORTUGUESA DE QUÍMICA
MAGALHÃES MCF (SCIENTIFIC ORGANISING COMMITTEE)
UNIVERSITY OF MINHO, PORTUGAL, 08-10 NOV 2007

7ª CONFERÊNCIA DE QUÍMICA INORGÂNICA
CAVALEIRO AMV (SCIENTIFIC ORGANISING COMMITTEE)
FÁTIMA, PORTUGAL, 30 NOV-01 DEC 2007

DYPROSO XXXI, XXXI INTERNATIONAL SYMPOSIUM ON DYNAMICAL PROPERTIES OF SOLIDS
VILARINHO PM (PROGRAMME COMMITEE)
PORTO, PORTUGAL, 25-29 SEPT 2007

ELECTROCERAMICA 2007-VIII NATIONAL MEETING
MARQUES FMB,VILARINHO P (CONFERENCE CHAIR), COSTA E, CARLOS L, ABRANTES JCC, KHARTON V, WU A, KHOLKIN A (LOCAL ORGANIZING COMMITTEE), VIEIRA J, FRADE JR (SCIENTIFIC COMMITTEE)
AVEIRO, PORTUGAL, 24-26 JUN 2007

E-MRS WASAW 2007
PINNA N (ORGANISING COMMITTEE)
WARSAW, POLAND, 17-21 SEPT 2007

EUROCLAYS 2007
LABRINCHA JA (SCIENTIFIC ORGANISING COMMITTEE)
AVEIRO, PORTUGAL, 22-27 JUL 2007

II CONGRESSO NACIONAL DE ARGAMASSAS DE CONSTRUÇÃO
LABRINCHA JA (SCIENTIFIC ORGANISING COMMITTEE)
LISBOA, PORTUGAL, 22-23 NOV 2007

IMPRES-INTERNATIONAL SYMPOSIUM ON INNOVATIVE MATERIALS FOR PROCESSES IN ENERGY SYSTEMS
FRADE JR (INTERNATIONAL SCIENTIFIC COMMITTEE)
KYOTO, JAPAN, 28-31 OCT 2007

ISDS 07 - 2ND INTERNATIONAL SYMPOSIUM 'MICRO- AND NANOSCALE DOMAIN STRUCTURING IN FERROELECTRICS'
KHOLKIN A (INTERNATIONAL SCIENTIFIC COMMITTEE)
EKATERINBURG, RUSSIA, 22-26 AUG 2007

IV JORNARDAS CICECO
WU A, CARLOS L, PEREIRA S, BRAGA S (ORGANISING COMMITTEE)
AVEIRO, PORTUGAL, 11-12 JAN 2007

MATERIAIS 2007 - GLOBAL MATERIALS FOR THE XXI CENTURY: CHALLENGES TO ACADEMIA AND INDUSTRY
VILARINHO PM (SCIENTIFIC ORGANISING COMMITTEE)
PORTO, PORTUGAL, 25-27 APR 2007

SSI-16, THE 16TH INTERNATIONAL CONFERENCE ON SOLID STATE IONICS
MARQUES FMB (INTERNATIONAL SCIENTIFIC ADVISORY COMMITTEE)
SHANGHAI, CHINA, 01-06 JUL 2007

THE SEVENTH STUDENTS' MEETING: PROCESSING AND APPLICATION OF CERAMICS
KHARTON V (INTERNATIONAL SCIENTIFIC COMMITTEE)
NOVI SAD, SERBIA, 06-07 DEC 2007

VIII LATIN AMERICAN WORKSHOP ON MAGNETISM, MAGNETIC MATERIALS AND THEIR APPLICATIONS
REIS MS (CHAIRMAN)
RIO DE JANEIRO, BRASIL, 12-16 AUG 2007

Courses, Seminars and Trainning Programmes

ADVANCED CHARACTERIZATION OF INTEGRATED FERROELECTRICS, COURSE ON 19TH INTERNATIONAL SYMPOSIUM ON INTEGRATED FERROELECTRICS
KHOLKIN A
BORDEUS, FRANÇA, 08 MAY 2007

COLOIDES, SUPERFÍCIES E INTERFASES: CURSO DE POSGRADUAÇÃO REALIZADO PELA IDPoR
GANDINI A
UNIVERSITY OF AVEIRO, PORTUGL, 2007
http://idpor.ciceco.ua.pt/

EMMS – EUROPEAN MASTER IN MATERIALS SCIENCE (LOCAL COORDINATION)
BARROS-TIMMONS A; NOGUEIRA H
UNIVERSITY OF AVEIRO, PORTUGAL, 2007,
http://www.ua.pt/ipp/emms

INTEGRATED PIEZOELECTRIC MATERIALS, COURSE ON 1ST WINTER SCHOOL FAME: WP5 "NEW ARCHITECTURES FOR PASSIVE ELECTRONICS"
KHOLKIN AL
LA CLUSAZ, FRANÇA, 14-21 JAN 2007

ACADEMIA DE VERÃO | SUMMER SCHOOL
RIBEIRO-CLARO P, GOODFELLOW B
19 JUL 2007, UNIVERSITY OF AVEIRO

OLIMPÍADAS DE QUÍMICA JÚNIOR
RIBEIRO-CLARO P, GOODFELLOW B, CAVALEIRO A, CARAPUÇA H, SANTOS TM
21 APR 2007, UNIVERSITY OF AVEIRO

OLIMPÍADAS DE QUÍMICA – SEMIFINAL
RIBEIRO-CLARO P
03 MAR 2007, UNIVERSITY OF AVEIRO

OLIMPÍADAS DE QUÍMICA – FINAL
RIBEIRO-CLARO P
05 MAY 2007, UNIVERSITY OF AVEIRO

QUÍMICA EM ESPECTÁCULO | CHEMISTRY-IN-A-SHOW
DEMONSTRATIONS OF CHEMISTRY AND MATERIALS TO SECONDARY SCHOOL STUDENTS
RIBEIRO-CLARO P
SEMANA DA CIÊNCIA E DA TECNOLOGIA
19-24 NOV 2007, UNIVERSITY OF AVEIRO

SERÁ QUE O OCEANO TEM ALGUM EFEITO NO AQUECIMENTO GLOBAL? ONDE ESTÁ A QUÍMICA?
MAGALHÃES MCF
SEMANA DA CIÊNCIA E DA TECNOLOGIA
19-24 NOV 2007, UNIVERSITY OF AVEIRO

LEGO-QUÍMICA: A NANOTECNOLOGIA NAS NOSSAS MÃOS
TRINDADE T
SEMANA DA CIÊNCIA E DA TECNOLOGIA
19-24 NOV 2007, UNIVERSITY OF AVEIRO

POLÍMEROS SINTÉTICOS E NATURAIS
GANDINI A
SEMANA DA CIÊNCIA E DA TECNOLOGIA
19-24 NOV 2007, UNIVERSITY OF AVEIRO

PMATE (NATIONAL MATHS CONTEST FOR KIDS)
RIBEIRO-CLARO P, GOODFELLOW B
02-04 MAY 2007, UNIVERSITY OF AVEIRO

II JORNADAS DE CIÊNCIA (SCIENCE FAIR)
22 FEB 2007, SCHOOL EXTERNATO DELFIM FERREIRA
SEMANA DO PATRONO (SCIENCE FAIR)
08 MAR 2007, SCHOOL ES HOMEM CRISTO

PUBLIC DEMONSTRATION CICECO@FÁBRICA:
"CICECO – FROM THE CHEMISTRY SHOW TO THE WORLD OF MATERIALS"
RIBEIRO-CLARO P, GOODFELLOW B, LABRINCHA J
SEMANA DA CIÊNCIA E DA TECNOLOGIA
14 APR 2007, FÁBRICA CENTRO DE CIÊNCIA VIVA

RECEPTION OF FIRST YEAR DQ-UA STUDENTS
RIBEIRO-CLARO P
25 SEP 07, UNIVERSITY OF AVEIRO
SCHOOL VISIT TO DQ-UA
RIBEIRO-CLARO P
30 NOV 2007, 12 DEZ 2007, UNIVERSITY OF AVEIRO

PROJECT COOPERATION WITH FÁBRICA CENTRO DE CIÊNCIA VIVA DE AVEIRO
RIBEIRO-CLARO P, GOODFELLOW B, CARDOSO M (GRANT)

A QUÍMICA DO AMOR | THE CHEMISTRY OF LOVE
CAFÉ DA CIÊNCIA | SCIENCE CAFÉ
RIBEIRO-CLARO P
19 NOV 2007, UNIVERSITY OF AVEIRO

IMPACIÊNCIAS
CAFÉ DA CIÊNCIA | SCIENCE CAFÉ
RIBEIRO-CLARO P
15 FEB 2007, FÁBRICA CIÊNCIA VIVA

POLÍMEROS SINTÉTICOS E NATURAIS
GANDINI A
2007, FÁBRICA CIÊNCIA VIVA

DO NAUFRÁGIO DO PRESTIGE À CASINHA DE CHOCOLATE DE JOÃO E MARIA: UM PASSEIO À LUZ DA VELA
COUTINHO JAP
17 MAY 2007, FÁBRICA CENTRO DE CIÊNCIA VIVA

NANOESTRUTURAS QUÂNTICAS
CIÊNCIA EM PORTUGAL - CIÊNCIA 2007
TRINDADE T, PEREIRA S
12 APR 2007, FUNDAÇÃO CALOUSTE GULBENKIAN- LISBOA

5DEDQ, 5TH MEETING EDUCATION IN CHEMISTRY
RIBEIRO-CLARO P
8 NOVEMBER 2007, UNIVERSIDADE DO MINHO

"QUÍMICA NAS ESCOLAS" - ACTIVIDADES PARA PROFESSORES DO ENSINO SECUNDÁRIO (11º ANO) - ACTIVIDADES LABORATORIAIS - ACTIVIDADES PRÁTICAS DE SALA DE AULA RELACIONADAS COM "AMONÍACO E SEUS COMPOSTOS" - PREPARAÇÃO DE UM COMPOSTO COM MOLÉCULAS DE NH3 COORDENADAS A UM CENTRO METÁLICO: - SÍNTESE DE UM COMPOSTO DE COORDENAÇÃO-ACÇÃO DE FORMAÇÃO E MATERIAL DE APOIO
SANTOS TM
2007

ACÇÕES DE DIVULGAÇÃO CIENTÍFICA EM ESCOLAS DO ENSINO SECUNDÁRIO
FRADE J
2007

COMENTÁRIOS AO FILME "NANOTECNOLOGIA"
TRINDADE T
19 AUG 2007, MERCADO MUNICIPAL DE CAXINAS CENTRO CIÊNCIA VIVA DE VILA DO CONDE

O PROCESSO DE BOLONHA E A OFERTA PEDAGÓGICA
FIGUEIREDO FM
SEMANA DA EUROPA
2007, ESCOLA SECUNDÁRIA DA LOURINHÃ, LOURINHÃ

ORGANIZAÇÃO DE ACÇÕES DE FORMAÇÃO PARA PROFESSORES DO ENSINO SECUNDÁRIO, NO ÂMBITO DA PLATAFORMA QUIMIMATER
FRADE F
2007

ORGANIZAÇÃO DE UMA VISITA DE ESTUDO AO LABORATÓRIO DO CICECO, DE ALUNOS DO 12º ANO, DA ÁREA DE CIÊNCIAS. O INTERESSE DOS VISITANTES RECAÍA NA VISUALIZAÇÃO DE TÉCNICAS CROMATOGRÁFICAS GC E HPLC E NA APRESENTAÇÃO DE ESTUDOS CIENTÍFICOS DESENVOLVIDOS NO LABORATÓRIO DO CICECO ONDE ESTAS TÉCNICAS SÃO PERTINENTES
VALENTE A
2007

ORIENTAÇÃO DE NÚCLEOS DE ESTÁGIOS PEDAGÓGICOS EM ESCOLAS BÁSICAS E SECUNDÁRIAS
SANTOS TM
2007

OS NANOMATERIAIS' - PALESTRA NA ESCOLA SECUNDÁRIA SERAFIM LEITE- S. J. MADEIRA
TRINDADE T
2007

SEMANA DA PRÁTICA PEDAGÓGICA
SANTOS TM
MAY 2007, UNIVERSITY OF AVEIRO

SCIENTIFIC PROMOTION OF THE ACTIVITIES OF CHEMESTRY DEPARTMENT
TIMMONS AB
2007

SALCIÊNCIA - PROJECTO CIÊNCIA VIVA
MAGALHÃES MCF
2007, AGÊNCIA NACIONAL PARA A CULTURA CIENTÍFICA E TECNOLÓGICA

PARTICIPAÇÃO COM PROTÓTIPOS DE "MOSAICOS DE ESCÓRIAS" NO PROJECTO DE ECO-DESIGN REMADE IN PORTUGAL
FERNANDES MHV
2007, NAVE DA ESTUFA FRIA (LX) E SERRALVES (PORTO)

RADIO PROGRAMMES
EXPLICAÇÃO QUÍMICA DA ROLHA DE CHAMPANHE E DO FOGO DE ARTIFÍCIO | CHEMISTRY OF FIREWORKS
TSF RADIO: PROGRAMME "EUREKA – SCIENCE AND TECHNOLOGY"
RIBEIRO-CLARO P
06 JAN 2007

DIA MUNDIAL DO SONO | CHEMISTRY OF SLEEP
TSF RADIO: PROGRAMME "EUREKA – SCIENCE AND TECHNOLOGY"
RIBEIRO-CLARO P
24 MAR 2007

BIOMATERIAIS | BIOMATERIALS
TSF RADIO: PROGRAMME "EUREKA – SCIENCE AND TECHNOLOGY"
FERNANDES H

RECICLAGEM | RECYCLING
TSF RADIO: PROGRAMME "EUREKA – SCIENCE AND TECHNOLOGY"
FERNANDES H
2007

MATERIAIS DE MUDANÇA DE FASES
TSF RADIO: PROGRAMME "EUREKA – SCIENCE AND TECHNOLOGY"
COUTINHO J
02 JUN 2007

RÚBRICA EDUCAÇÃO, CIÊNCIA E SOCIEDADE
ANTENA 1 RADIO: PROGRAMME "CLICK – SCIENCE AND TECHNOLOGY"
PEDROSA J
10 NOV 2007

RÚBRICA QUÍMICA DAS COISAS | 3 MINUTES APPOINTMENT "CHEMISTRY OF THINGS"
ANTENA 1 RADIO: PROGRAMME "CLICK – SCIENCE AND TECHNOLOGY"
RIBEIRO-CLARO P
17 NOV 2007; 15 DEC 2007

REPORTAGEM NANOTECNOLOGIA EM DIÁLOGO COM A NATUREZA
ANTENA 1 RADIO: PROGRAMME "CLICK – SCIENCE AND TECHNOLOGY"
TRINDADE T, LÁZARO C
24 NOV 2007

RÚBRICA EDUCAÇÃO, CIÊNCIA E SOCIEDADE
PEDROSA J
01 DEC 2007

ESPECIAL NATAL – CURIOSIDADES | CURIOSITIES
ANTENA 1 RADIO: PROGRAMME "CLICK – SCIENCE AND TECHNOLOGY"
RIBEIRO-CLARO P
22 DEC 2007

ESPECIAL ANO NOVO – ROLHA DE CHAMPANHE E FOGO DE ARTIFÍCIO | CHEMISTRY OF NEW YEAR
ANTENA 1 RADIO: PROGRAMME "CLICK – SCIENCE AND TECHNOLOGY"
RIBEIRO-CLARO P
29 DEC 2007

RADIO INTERVIEWS
CAFÉ COM / OLIMPÍADAS DE QUÍMICA JÚNIOR
VOZ DE VAGOS 88.8 FM
RIBEIRO-CLARO P
20 APR 2007

CHEMISTRY IN A MIDNIGHT SUMMER
VOZ DE VAGOS 88.8 FM
RIBEIRO-CLARO P
18 JUL 07

TV PROGRAMME
BIOMATERIAIS | BIOMATERIALS
3810 - UA (RTP 2)
FERNANDES H

RECICLAGEM | RECYCLING
3810 - UA (RTP 2)
FERNANDES H

SACT: EXPERIENCIAS DE QUÍMICA
3810 - UA (RTP 2)
RIBEIRO-CLARO P, GOODFELLOW B
04 DEC 2007

NANOQUÍMICA
3810 - UA (RTP 2)
TRINDADE T
02 MAY 2007; 17 APR 2007

RECICLAGEM | RECYCLING
BIOESFERA (RTP N)
FERNANDES H

A QUÍMICA DOS NANO-GLUTÕES ECOLÓGICOS
ESTÁGIO CIENTÍFICO DO PROGRAMA CIÊNCIA VIVA
TRINDADE T
JUL 2007, UNIVERSITY OF AVEIRO

MEMBER OF THE EDITORIAL BOARD

"PROCESSING AND APPLICATION OF CERAMICS" JOURNAL
KHARTON V
2007, FACULTY OF TECHNOLOGY, UNIVERSITY OF NOVI SAD, SERBIA

MATERIALS LETTERS (ELSEVIER)
KHARTON V
2007

THE OPEN CONDENSED MATTER PHYSICS JOURNAL (BENTHAM SCIENCE PUBL)
KHARTON V
2007

"HOLZFORSCHUNG" - INTERNATIONAL JOURNAL OF THE BIOLOGY, CHEMISTRY, PHYSICS AND TECHNOLOGY OF WOOD (WALTER DE GRUYTER)
EVTYUGIN D
2004-2008, BERLIN, GERMANY

JOURNAL WOOD CHEMISTRY AND TECHNOLOGY - INTERNATIONAL JOURNAL OF THE WOOD CHEMISTRY AND TECHNOLOGY (MARCEL DEKKER, INC.)
EVTYUGIN D
2007-2012, NEW YORK, USA

TOPICAL EDITOR OF THE JOURNAL OF SOLID STATE ELECTROCHEMISTRY (SPRINGER)
KHARTON V
2007

MEMBER OF EU COST E41 ACTION "ANALYTICAL TOOLS WITH APPLICATIONS FOR WOOD AND PULPING CHEMISTRY" (2004-2007)
EVTYUGIN D

SECTION 5
Projects

Projects Terminated

INTERNATIONAL PROJECTS | UA: PARTNER
DOLCETA - DEVELOPMENT OF ON-LINE CONSUMER EDUCATION TOOLS FOR ADULTS
PRINCIPAL RESEARCHER: MARIA CLARA FERREIRA MAGALHÃES
BEGINNING DATE: 01-12-2003 | 36 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 21.268,00

EVG1-CT-2002-00068 | E-ECORISK – A REGIONAL ENTERPRISE NETWORK DECISION SUPPORT SYSTEM FOR ENVIRONMENTAL RISK AND DISASTER MANAGEMENT OF LARGE SCALE INDUSTRIAL SPILLS
PRINCIPAL RESEARCHER: MARIA CLARA FERREIRA MAGALHÃES
BEGINNING DATE: 01-01-2004 | 40 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): -

IS-390 | STUDIES OF COLOSSAL MAGNETORESISTIVE OXIDES WITH RADIOACTIVE ISOTOPES
PRINCIPAL RESEARCHER: VITOR BRÁS DE SEQUEIRA AMARAL
BEGINNING DATE: 01-01-2005 | 36 MONTH
FUNDING: ISOLDE/CERN| UA VALUE (€): -

MNAA - MATERIALS NETWORK FOR THE ATLANTIC AREA | NETWORKED CENTRE OF EXCELLENCE IN MATERIALS FOR THE ECONOMIC DEVELOPMENT OF THE ATLANTIC AREA
PRINCIPAL RESEARCHER: JOÃO CARLOS MATIAS CELESTINO GOMES DA ROCHA
BEGINNING DATE: 01-01-2004 | 36 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 521.109,49

RFS-CR-04031-PRIMEFORM | FORMABILITY AND SELF-REPAIR PROPERTIES OF ADVANCED WELDABLE PRIMERS
PRINCIPAL RESEARCHER: MÁRIO GUERREIRO DA SILVA FERREIRA
BEGINNING DATE: 01-07-2004 | 36 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 148.600,00

NATIONAL PROJECTS | UA: COORDINATOR
CIÊNCIA VIVA | OLIMPÍADAS DE QUÍMICA JÚNIOR 2007
PRINCIPAL RESEARCHER: PAULO JORGE DE ALMEIDA RIBEIRO CLARO
BEGINNING DATE: 02-01-2006 | 22 MONTH
FUNDING: FCT | UA VALUE (€): 7.700,00

F-20/07 | UMA NOVA CLASSE DE SONDAS NANOMÉTRICAS PARA IMAGEM POR RESSONÂNCIA MAGNÉTICA E IMAGEM ÓPTICA. DA SÍNTESE AOS TESTES IN VITRO
PRINCIPAL RESEARCHER: LUÍS ANTÓNIO FERREIRA MARTINS DIAS CARLOS
BEGINNING DATE: 01-01-2006 | 24 MONTH
FUNDING: FCT | UA VALUE (€): 4.000,00

POCI/AMB/59408/2004 | REUSE AND IMMOBOLISATION OF INDUSTRIAL WASTES BY GEOPOLYMERISATION: NEW CONSTRUCTION ARTEFACTS
PRINCIPAL RESEARCHER: JOÃO ANTÓNIO LABRINCHA BATISTA
BEGINNING DATE: 01-01-2006 | 24 MONTH
FUNDING: FCT | UA VALUE (€): 47.280,00

POCI/CTM/59075/2004 | NEW ORGANIC/INORGANIC HYBRIDS FOR INTEGRATED OPTICS
PRINCIPAL RESEARCHER: MARIA RUTE DE AMORIM E SÁ FERREIRA ANDRÉ
BEGINNING DATE: 01-04-2005 | 24 MONTH
FUNDING: FCT | UA VALUE (€): 39.915,00

POCI/CTM/58863/2004 | LUMINESCENT LANTHANIDE SILICATE SYNTHESIS USING LANTHANIDE COMPLEXES AS STRUCTURE DIRECTING AGENTS
PRINCIPAL RESEARCHER: ANTÓNIO MOREIRA DOS SANTOS
BEGINNING DATE: 01-05-2005 | 24 MONTH
FUNDING: FCT | UA VALUE (€): 39.271,00

POCTI/CTM/47285/2002 | NOVEL BST DIELECTRIC FILMS FOR ULTRA HIGH DENSITY DRAMS
PRINCIPAL RESEARCHER: PAULA MARIA LOUSADA SILVEIRINHA VILARINHO
BEGINNING DATE: 20-02-2004 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 67.534,00

POCI/CTM/61071/2004 | NANO-SCALE INVESTIGATION OF FATIGUE OF FERROELECTRIC THIN FILMS
PRINCIPAL RESEARCHER: AIYING WU
BEGINNING DATE: 01-08-2005 | 24 MONTH
FUNDING: FCT | UA VALUE (€): 72.477,00

POCI/CTM/59197/2004 | DEVELOPMENT OF NEW INTERSTITIAL OXIDE-ION CONDUCTORS FOR EFFECTIVE OXYGEN SEPARATION AND CONVERSION OF THE HYDROCARBONS
PRINCIPAL RESEARCHER: YEVGENIY (EUGENE) NAUMOVICH
BEGINNING DATE: 01-01-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 53.610,00

POCI/CTM/59727/2004 | CORE-SHELL CERAMIC MEMBRANES WITH NANO-SIZED GRAINS FOR OXIGEN SEPARATION AND SYN-GAS PRODUCTION
PRINCIPAL RESEARCHER: FILIPE MIGUEL H. LEBRE R. FIGUEIREDO
BEGINNING DATE: 01-07-2005 | 24 MONTH
FUNDING: FCT | UA VALUE (€): 65.000,00

POCI/CTM/60761/2004 | SURFACE REACTIVITY OF TIO2-CONTAINING GLASSES IN SIMULATED PHYSIOLOGICAL SOLUTIONS
PRINCIPAL RESEARCHER: MARIA HELENA FIGUEIRA VAZ FERNANDES
BEGINNING DATE: 01-06-2005 | 24 MONTH
FUNDING: FCT | UA VALUE (€): 43.000,00

POCTI/EQU/47533/2002 | SUPERCRITICAL FLUID EXTRACTION OF GRAPE SEED OIL: ENHANCEMENT OF RECOVERY USING ENZYMATIC PRE-TREATMENT OF SEED
PRINCIPAL RESEARCHER: CARLOS MANUEL SANTOS SILVA
BEGINNING DATE: 01-02-2004 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 20.000,00

POCI/EQU/58239/2004 | EQUILIBRIUM AND INTERFACIAL PROPERTIES OF WATER + OIL SYSTEMS
PRINCIPAL RESEARCHER: ANTÓNIO JOSÉ NASCIMENTO QUEIMADA
BEGINNING DATE: 01-01-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 45.000,00

POCI/QUI/56109/2004 | NEW OXOMETAL COMPOUNDS WITH TAILORED CATALYTIC PROPERTIES
PRINCIPAL RESEARCHER: ISABEL MARIA SOUSA GONÇALVES
BEGINNING DATE: 01-01-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 31.700,00
PROGRAMA ESTÍMULO À EXCELÊNCIA - JOSÉ F. FERREIRA
PRINCIPAL RESEARCHER: JOSÉ MARIA DA FONTE FERREIRA
BEGINNING DATE: 03-08-2005 | 24 MONTH
FUNDING: FCT | UA VALUE (€): 10.000,00

REAL - SPACE CHARACTERIZATION OF FERROELECTRIC NANOSTRUCTURES
PRINCIPAL RESEARCHER: PAULA MARIA LOUSADA SILVEIRINHA VILARINHO PROPONENTE
BEGINNING DATE: 01-01-2007 | 12 MONTH
FUNDING: FLAD | UA VALUE (€): 15.000,00

NATIONAL PROJECTS | UA: PARTNER
POCI/CTM/57536/2004 | NEW METHODOLOGY FOR THE PRODUCTION OF LIGHT WEIGHT INTERMETALLIC MATRIX COMPOSITES WITH IMPROVED MECHANICAL PROPERTIES
PRINCIPAL RESEARCHER: RUI RAMOS FERREIRA E SILVA
BEGINNING DATE: 01-06-2005 | 30 MONTH
FUNDING: FCT | UA VALUE (€): 18.600,00

POCTI/CTM/46270/2002 | QUANTITATIVE ANALYSIS OF THE SHEAR EFFECTS ON THE SOLIDIFICATION OF POLYMERS WITH A SHEAR-DSC
PRINCIPAL RESEARCHER: JOSÉ JOAQUIM COSTA CRUZ PINTO
BEGINNING DATE: 01-10-2004 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 5.938,00

OTHER PROJECTS, COOPERATION AGREEMENT AND CONTRACTS | UA: PARTNER
E-75/05 | ESTUDO COMPARATIVO DO COMPORTAMENTO "IN VITRO" DE VIDROS DO SISTEMA SI-CA-P-MG, EM ESPÉCIMES MONOLÍTICOS E NA FORMA DE FILMES
PRINCIPAL RESEARCHER: MARIA HELENA FIGUEIRA VAZ FERNANDES
BEGINNING DATE: 01-01-2005 | 24 MONTH
FUNDING: CRUP | VALUE (€): 1.100,00

MATERIAIS HÍBRIDOS ORGÂNICOS-INORGÂNICOS PARA APLICAÇÕES EM ÓPTICA INTEGRADA
PRINCIPAL RESEARCHER: LUÍS ANTÓNIO FERREIRA MARTINS DIAS CARLOS
BEGINNING DATE: 01-01-2005 | 24 MONTH
FUNDING: GRICES

PE067 | INTERACÇÃO TINTA PAPEL
PRINCIPAL RESEARCHER: DMITRY VICTOROVITCH EVTYUGIN
BEGINNING DATE: 15-07-2005 | 24 MONTH
FUNDING: RAIZ | UA VALUE (€): 25.000,00

SUB-PROJECTO RECICLAGEM – CASA DO FUTURO
PRINCIPAL RESEARCHER: VICTOR MIGUEL DE SOUSA FERREIRA
BEGINNING DATE: 01-03-2006 | 12 MONTH
FUNDING: AVEIRODOMUS | UA VALUE (€): 60.500,00

SUB-PROJECTO REVESTIMENTOS – CASA DO FUTURO
PRINCIPAL RESEARCHER: VICTOR MIGUEL DE SOUSA FERREIRA
BEGINNING DATE: 01-03-2006 | 12 MONTH
FUNDING: AVEIRODOMUS | UA VALUE (€): 53.845,00

OTHER PROJECTS, COOPERATION AGREEMENT AND CONTRACTS | UA: COORDINATOR

APPLICATION OF NMR METHODS FOR THE CHARACTERIZATION AND QUALITY CONTROL OF BEER
PRINCIPAL RESEARCHER: ANA MARIA PISSARRA COELHO GIL
BEGINNING DATE: 01-04-2005 | 24 MONTH
FUNDING: UNICER-BEBIDAS DE PORTUGAL, SGPS, S.A. | VALUE (€): 12.500,00

CARACTERIZAÇÃO E DESENVOLVIMENTO DE AGLOMERANTES PARA A INDÚSTRIA DE MÓS ABRASIVOS
PRINCIPAL RESEARCHER: RUI RAMOS FERREIRA E SILVA
BEGINNING DATE: 01-01-2006 | 24 MONTH
FUNDING: DRAGÃO ABRASIVOS | UA VALUE (€): 10.800,00

EQUILÍBRIO DE FASES E PROCESSOS DE SEPARAÇÃO DE GORDURAS
PRINCIPAL RESEARCHER: JOÃO MANUEL DA COSTA E ARAÚJO PEREIRA COUTINHO
BEGINNING DATE: 01-01-2006 | 24 MONTH
FUNDING: GRICES | UA VALUE (€): 5.000,00

INTERNATIONAL PROJECTS | UA: COORDINATOR

BIO-TRIBODIAM - DLC AND CVD DIAMOND COATED SI3N4 CERAMICS FOR TRIBOLOGICAL AND BIOMEDICAL PURPOSES
PRINCIPAL RESEARCHER: RUI RAMOS FERREIRA E SILVA
BEGINNING DATE: 01-04-2006 | 24 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 129.870,31

INTAS-05-1000008-8091 | POLARIZATION-DRIVEN SELF-ASSEMPLY OF ORGANICS AND BIOMATERIALS USING ULTRATHIN FERROELECTRIC POLYMERS
PRINCIPAL RESEARCHER: ANDREI KHOLKIN
BEGINNING DATE: 01-11-2006 | 30 MONTH
FUNDING: INTAS | UA VALUE (€): 150.000,00

GRICES 4.1.1 CNR | DEVELOPMENT AND CHARACTERIZATION OF NOVEL MULTIFERROIC CERAMICS AND COMPOSITES
PRINCIPAL RESEARCHER: ANDREI KHOLKIN
BEGINNING DATE: 01-01-2007 | 24 MONTH
FUNDING: GRICES | UA VALUE (€): 10.000,00

MAEIF-CT-2006-041632 - MULTIFERRO-SOL-GEL | MULTIFERROIC NANOSTRUCTURES: A NON-AQUEOUS SOL-GEL APPROACH (MULTIFERRO-SOL-GEL)
PRINCIPAL RESEARCHER: NICOLA ALLESSANDRO PINNA
BEGINNING DATE: 01-12-2006 | 24 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 138.246,64

MULTICERAL-MULTIFUNCTIONAL CERAMICS LAYERS WITH HIGH ELECTRO-MAGNETOELASTIC COUPLIN IN COMPLEX GEOMETRIES
PRINCIPAL RESEARCHER: ANDREI KHOLKIN
BEGINNING DATE: 01-11-2006 | 36 MONTH
FUNDING: EUROPEAN COMISSION | UA VALUE (€): 1.549.740,00

NANOSCALE CHARACTERIZATION OF FERROELECTRIC FULMS AND DEVICES
PRINCIPAL RESEARCHER: ANDREI KHOLKIN
BEGINNING DATE: 01-01-2008 | 24 MONTH
FUNDING: GRICES | UA VALUE (€): -

INTERNATIONAL PROJECTS | UA: PARTNER

11783-2 MULTIPROTECT | ADVANCED ENVIRONMENTALLY FRIENDLY MULTIFUNCTIONAL CORROSION PROTECTION BY NANOTECHNOLOGY
PRINCIPAL RESEARCHER: MÁRIO GUERREIRO DA SILVA FERREIRA
BEGINNING DATE: 01-03-2005 | 48 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 282.203,00

COST 539 ACTION | ELECTROCERAMICS FROM NANOPOWDERS PRODUCED BY INNOVATIVE METHODS-ELENA
PRINCIPAL RESEARCHER: PAULA MARIA LOUSADA SILVEIRINHA VILARINHO
BEGINNING DATE: 01-03-2005 | 36 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): -

FP6 2004 NMP3/CT (NOE 500159) | NETWORK OF EXCELLENCE: FUNCTIONALISED ADVANCED MATERIALS AND ENGINEERING OF HYBRIDS AND CERAMICS (FAME)
PRINCIPAL RESEARCHER: JOÃO CARLOS MATIAS CELESTINO GOMES DA ROCHA
BEGINNING DATE: 01-10-2004 | 48 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 219.408,75

FP6 2002 NMP/1 (IP 500311-2) | SUSTAINPACK - INNOVATION AND SUSTAINABLE DEVELOPMENT IN THE FIBRE BASED PACKAGING VALUE CHAIN
PRINCIPAL RESEARCHER: CARLOS DE PASCOAL NETO
BEGINNING DATE: 01-06-2004 | 48 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 218.360,00

FP 7 - MULTI-LEVEL PROTECTION OF MATERIALS FOR VEHICLES BY 'SMART' NANOCONTAINERS
PRINCIPAL RESEARCHER: MIKHAIL ZHELUDKEVICH
BEGINNING DATE: 01-05-2008 | 48 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 824.769,00

NMP2-CT-2004-515960 ULCOS | ULTRA LOW CO2 STEELMAKING
PRINCIPAL RESEARCHER: JORGE MANUEL RIBEIRO FRADE
BEGINNING DATE: 01-09-2004 | 60 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 316.406,94

NMP3-CT-2007-032308 – NANOCOFC | NANOTECHNOLOGIES AND NANOSCIENCES, KNOWLEDGE BASED MULTIFUNCTIONAL MATERIALS, NEW PRODUCTION PROCESSES AND DEVICES
PRINCIPAL RESEARCHER: FERNANDO MANUEL BICO MARQUES
BEGINNING DATE: 01-11-2006 | 36 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 34.650,00

PREDICTION OF THE KINETICS OF SELF-REPAIRED OF FORMING INDUCED DEFECTS ON THIN FUNCTIONAL PRIMERS FOR ADVANCES AUTOMOTIVE APPLICATIONS
PRINCIPAL RESEARCHER: MIKHAIL ZHELUDKEVICH
BEGINNING DATE: 01-07-2008 | 36 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 160.341,00

STRP 033410 MATSILC | MATSILC-NOVEL MATERIALS FOR SILICATE BASED FUEL CELL
PRINCIPAL RESEARCHER: JORGE MANUEL RIBEIRO FRADE
BEGINNING DATE: 01-12-2006 | 36 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 252.000,00

WACHEUP - NEW CONCEPTS FOR UPGRADING PULP MILL WASTE STREAMS TO VALUES - ADDED CHEMICALS
PRINCIPAL RESEARCHER: CARLOS DE PASCOAL NETO
BEGINNING DATE: 01-06-2005 | 36 MONTH
FUNDING: EUROPEAN COMMISSION | UA VALUE (€): 255.000,00

NATIONAL PROJECTS | UA: COORDINATOR
FLAD 600-06/2006 | DEVELOPMENT AND CHARACTERIZATION OF NOVEL MULTIFERROIC MATERIALS AND STRUCTURES
PRINCIPAL RESEARCHER: ANDREI KHOLKIN
BEGINNING DATE: 01-01-2007 | 24 MONTH
FUNDING: FLAD | UA VALUE (€): 30.000,00

POCI/AMB/55939/2004 | MODIFIED ELECTRODES: FROM VERSATILE MODELS TO FUNCTIONAL DEVICES FOR STUDYING DYNAMIC SPECIATION IN THE ENVIRONMENT
PRINCIPAL RESEARCHER: HELENA MARIA CORREIA SEXAS CARAPUÇA
BEGINNING DATE: 01-01-2006 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 61.794,00

POCI/CTM/58570/2004 | NOVEL CERAMIC MEMBRANES FOR SYNTHESIS GAS PRODUCTION
PRINCIPAL RESEARCHER: VLADISLAV KHARTON
BEGINNING DATE: 01-05-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 64.000,00

POCI/CTM759449/2004 | NANODIAM - NANOCRYSTALLINE DIAMOND (NCD) FILMS ON SILICON NITRIDE CERAMICS FOR TRIBOLOGICAL APPLICATIONS
PRINCIPAL RESEARCHER: RUI RAMOS FERREIRA E SILVA
BEGINNING DATE: 16-08-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 53.760,00

POCI/CTM/59234/2004 | DEVELOPMENT OF NEW NANOSTRUCTURED HYBRID SOL-GEL COATINGS MODIFIED WITH ORGANIC INHIBITORS FOR CORROSION PROTECTION OF METALLIC SUBSTRATES
PRINCIPAL RESEARCHER: MÁRIO GUERREIRO DA SILVA FERREIRA
BEGINNING DATE: 01-07-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 53.800,00

POCI/CTM/58507/2004 | MULTIFUNCTIONAL ANIONIC CLAYS
PRINCIPAL RESEARCHER: MARTYN PILLINGER
BEGINNING DATE: 01-02-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 44.000,00

POCI/CTM/55648/2004 | PERIODIC MESOPOROUS ORGANIC-INORGANIC HYBRIDS
PRINCIPAL RESEARCHER: PAULA CELESTE DA SILVA FERREIRA
BEGINNING DATE: 01-05-2006 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 55.000,00

POCI/FP/81979/2007 | ESTUDO DE ÓXIDOS MAGNÉTICOS USANDO ISÓTOPOS RADIOACTIVOS NO ISOLDE-CERN
PRINCIPAL RESEARCHER: VITOR BRÁS DE SEQUEIRA AMARAL
BEGINNING DATE: 16-11-2007 | 12 MONTH
FUNDING: FCT | UA VALUE (€): 35.000,00

POCI/FP/63953/2005 | ESTUDOS DE ÓXIDOS MAGNÉTICOS APLICANDO ISÓTOPOS RADIOACTIVOS (ISOLDE-CERN)
PRINCIPAL RESEARCHER: VITOR BRÁS DE SEQUEIRA AMARAL
BEGINNING DATE: 01-02-2007 | 12 MONTH
FUNDING: FCT | UA VALUE (€): 35.000,00

POCI/QUI/58887/2004 | POLYOXOMETALATES: FORM DISCRETE CLUSTERS TO NETWORKS AND MATERIALS
PRINCIPAL RESEARCHER: HELENA ISABEL SEGURO NOGUEIRA
BEGINNING DATE: 01-09-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 57.500,00

POCI/QUI/56534/2004 | NANOSTRUCTURED HYBRID ORGANIC-INORGANIC ASSEMBLIES: DEVELOPMENT OF LAYER-BY-LAYER AND SINGLE LAYER HETEROPOLYTUNGSTATE MODIFIED ELECTRODES
PRINCIPAL RESEARCHER: HELENA MARIA CORREIA SEXAS CARAPUÇA
BEGINNING DATE: 01-09-2005 | 36MONTH
FUNDING: FCT | UA VALUE (€): 62.000,00

POCI/QUI/58377/2004 | NOVEL MULTIDIMENSIONAL LANTHANIDE-ORGANIC FRAMEWORKS: HYDROTHERMAL SYNTHESIS, STRUCTURAL CHARACTERISATION AND APPLICATIONS
PRINCIPAL RESEARCHER: FILIPE ALEXANDRE ALMEIDA PAZ
BEGINNING DATE: 01-10-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 59.000,00

POCI/V.5/A0067/2005 | PHOTOLUMINESCENCE-STRUCTURE RELATIONSHIP IN ORGANIC-INORGANIC HYBRIDS FOR OPTICAL APPLICATIONS
PRINCIPAL RESEARCHER: LUÍS ANTÓNIO FERREIRA MARTINS DIAS CARLOS
BEGINNING DATE: 01-08-2007 | 16 MONTH
FUNDING: FCT | UA VALUE (€): 58.520,60

PTDC/CTM/65667/2006 | SYNTHESIS AND CHARACTERIZATION OF MULTIFERROIC NANOSTRUCTURES SYNTHETISED VIA NOVEL NON-AQUEOUS SOL-GEL ROUTES
PRINCIPAL RESEARCHER: NICOLA ALLESSANDRO PINNA
BEGINNING DATE: 01-11-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 151.000,00

PTDC/CTM/73243/2006 | NANOSTRUCTURED PHOTOLUMINESCENT RARE-EARTH NANOTUBES AND MICROPOROUS SILICATES
PRINCIPAL RESEARCHER: JOÃO CARLOS MATIAS CELESTINO GOMES DA ROCHA
BEGINNING DATE: 01-12-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 60.456,00

PTDC/CTM/81442/2006 | ORIGEM DO ESTADO POLAR EM RELAXORES POR MICROSOCOPIA DA SONDA DE VARRIMENTO
PRINCIPAL RESEARCHER: ANDREI KHOLKIN
BEGINNING DATE: 15-05-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 119.724,00

PTDC/CTM/68614/2006 | ESTUDOS DA SOLIDIFICAÇÃO EM POLÍMEROS E NANOCOMPÓSITOS SOB ACÇÃO DE ESFORÇOS DE CORTE
PRINCIPAL RESEARCHER: ANDREI KHOLKIN
BEGINNING DATE: 01-12-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 153.100,00

PTDC/CTM/65632/2006 | SELF-HEALING PROTECTIVE COATING WITH 'INTELLIGENT' NANORESERVOIRS OF CORROSION INHIBITORS
PRINCIPAL RESEARCHER: MIKHAIL ZHELUDKEVICH
BEGINNING DATE: 01-03-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 157.200,00

PTDC/CTM/72318/2006 | ECOPIGMENTS - DEVELOPMENT OF NOVEL INORGANIC PIGMENTS FROM INDUSTRIAL WASTES
PRINCIPAL RESEARCHER: JOÃO ANTÓNIO LABRINCHA BATISTA
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 62.880,00

PTDC/QUI/65805/2006 | WATER NANODROPS IN MICROPOROUSE AND INORGANIC-ORGANIC HYBRID MATERIALS
PRINCIPAL RESEARCHER: JOÃO CARLOS MATIAS CELESTINO GOMES DA ROCHA
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 61.000,00

PTDC/QUI/67712/2006 | NANOQUÍMICA DE COMPÓSITOS MAGNÉTICOS/LUMINISCENTES PARA APLICAÇÕES DE DIAGNÓSTICO MÉDICO IN VITRO
PRINCIPAL RESEARCHER: TITO DA SILVA TRINDADE
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 40.900,00

PTDC/QUI/72584/2006 | PHOTOCATALYTIC REDUCTION OF CARBON DIOXIDE INTO VALUABLE HYDROCARBON PRODUCTS
PRINCIPAL RESEARCHER: PAULA CELESTE DA SILVA FERREIRA
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 41.200,00

PROGRAMA ESTÍMULO À EXCELÊNCIA - PAULA VILARINHO
PRINCIPAL RESEARCHER: PAULA MARIA LOUSADA SILVEIRINHA VILARINHO PROPONENTE
BEGINNING DATE: 14-02-2007 | 24 MONTH
FUNDING: FCT | UA VALUE (€): 10.000,00

POCI/QUI/56112/2004 | CATALYTIC CONVERSION OF CARBOHYDRATES INTO FURAN DERIVATIVES
PRINCIPAL RESEARCHER: ANABELA TAVARES AGUIAR VALENTE
BEGINNING DATE: 01-04-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 45.500,00

POCI/CTM/60288/2004 | DEVELOPMENT OF A NEW PHASE CHANGE MATERIAL COMPOSITE FOR ENERGY STORAGE AND THERMAL INSULATION
PRINCIPAL RESEARCHER: JOÃO MANUEL DA COSTA E ARAÚJO PEREIRA COUTINHO
BEGINNING DATE: 01-06-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 71.162,00

POCI/EQU/58152/2004 | SCREENING OF IONIC LIQUIDS FOR GAS SEPARATION
PRINCIPAL RESEARCHER: JOÃO MANUEL DA COSTA E ARAÚJO PEREIRA COUTINHO
BEGINNING DATE: 01-09-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 63.000,00

PTDC/QUE-FTT/65252/2006 | VAPOUS LIQUID EQUILIBRIUM OF PURE IONIC LIQUIDS AND THEIR MIXTURES WITH ORGANIC SOLVENTS
PRINCIPAL RESEARCHER: ISABEL MARIA DELGADO JANA MARRUCHO FERREIRA
BEGINNING DATE: 01-10-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 104.970,00

PTDC/EQU-ESI/68309/2006 | MODEL PREDICTIVE CONTROL FOR A PRESSURE SWING ADSORPTION UNIT WITH EXPERIMENTAL SUPPORT
PRINCIPAL RESEARCHER: FRANCISCO AVELINO DA SILVA FREITAS
BEGINNING DATE: 01-04-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 89.112,00

PTDC/CTM/64357/2006 | DESENVOLVIMENTO DE NOVAS FERRITES COM ESTRUTURA EM CAMADAS E CONDUTIVIDADE MISTA IÓNICA-E ELECTRÓNICA PARA APLICAÇÃO COMO FONTES ALTERNATIVAS DE ENERGIA
PRINCIPAL RESEARCHER: ANABELA TAVARES AGUIAR VALENTE
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): -

PPCTD/3599 | SHEAR INDUCED SOLIDIFICATION STUDIES IN POLYMERS AND NANOCOMPOSITES
PRINCIPAL RESEARCHER: JOSÉ MARTINS
BEGINNING DATE: 02-01-2008
FUNDING: FCT | UA VALUE (€): 150.000,00

PTDC/SAU-BEB/66896/2006 | IMPLANTABLE SCAFFOLDS FOR LOCAL OSTEO-SARCOMA CHEMOTHERAPY
PRINCIPAL RESEARCHER: RUI NUNES CORREIA
BEGINNING DATE: 01-09-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 161.200,00

PTDC/QUI/64203/2006 | STRUCTURAL AND FUNCTIONAL STUDIES OF THE SOUL/HBP FAMILY OF HEME-BINDING PROTEINS
PRINCIPAL RESEARCHER: BRIAN JAMES GOODFELLOW
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 55.950,00

PTDC/QUI/68017/2006 | METABOLIC PROFILING AND BIOCHEMICAL DIFFERENTIATION OF HUMAN LUNG TUMOURS BY NUCLEAR MAGNETIC RESONANCE (NMR) METHODS
PRINCIPAL RESEARCHER: IOLA MELISSA FERNANDES DUARTE
BEGINNING DATE: 15-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 59.200,00

POCI/HEC/57890/2004 | STUDY OF COMPATIBLE MORTARS FOR THE PRESERVATION OF THE BUILT HERITAGE
PRINCIPAL RESEARCHER: VICTOR MIGUEL DE SOUSA FERREIRA
BEGINNING DATE: 01-09-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 47.472,00

PTDC/ECM/72104/2006 | ESTUDO DE ARGAMASSAS FUNCIONAIS PARA UMA CONSTRUÇÃO SUSTENTÁVEL
PRINCIPAL RESEARCHER: VICTOR MIGUEL DE SOUSA FERREIRA
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): -

POCI/CTM/60207/2004 | SIMULTANEOUS PRECIPITATION AND IN SITU STABILISATION OF CALCIUM PHOSPHATE POWDERS FOR BIOMEDICAL APPLICATIONS IN BONE REPAIR AND CONTROLLED DRUG DELIVERY SYSTEMS
PRINCIPAL RESEARCHER: JOSÉ MARIA DA FONTE FERREIRA
BEGINNING DATE: 01-06-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 29.510,40

NATIONAL PROJECTS | UA: PARTNER

POCI/CTM/58183/2004 | IMMOBILIZED PHOTOSENSITIZER AS NEW MATERIALS IN WATER TREATMENT
PRINCIPAL RESEARCHER: JOSÉ ABRUNHERO CAVALEIRO | JOÃO ROCHA; ZHI LIN; JOSÉ RAINHO
BEGINNING DATE: 01-09-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 80.000,00

POCI/EQU/59345/2004 | DEVELOPMENT OF A FIXED SITE CARRIER CERAMIC ULTRAMICROPOROUS MEMBRANE REACTOR FOR THE SELECTIVE SEPARATION AND OXIDATION OF CARBON MONOXIDE TO CARBON DIOXIDE
PRINCIPAL RESEARCHER: ZHI LIN
BEGINNING DATE: 01-12-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 26.100,00

POCI/EQU/59344/2004 | DEVELOPMENT OF A FIXED SITE CARRIER CERAMIC ULTRAMICROPOROUS MEMBRANE AND CATALYTIC MEMBRANE REACTOR FOR OLEFINS SEPARATION/PURIFICATION
PRINCIPAL RESEARCHER: ZHI LIN
BEGINNING DATE: 01-12-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 29.580,00

PTDC/FIS/65233/2006 | TERNARY AND QUATERNARY NITRIDE ALLOYS FOR LATTICE MATCHES HETEROSTRUCTURES: NOVEL MATERIALS FOR HIGH EFFICIENCY FIELD EFFECT TRANSISTORS AND OPTOELECTRONIC DEVICES
PRINCIPAL RESEARCHER: SÉRGIO MANUEL SOUSA PEREIRA
BEGINNING DATE: 01-07-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 59.520,00

PTDC/QUE-ERQ/66045/2006 | USE OF MEMBRANE REACTORES IN THE WATER-GAS SHIFT REACTION
PRINCIPAL RESEARCHER: ZHI LIN
BEGINNING DATE: 01-09-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 25.919,00

PTDC/QUI/71198/2006 | ANSA-BRIDGED ORGANORHENIUM(VII) OXIDE AND THEIR APPLICATION AS HOMOGENEOUS AND HETEROGENEOUS CATALYSTS
PRINCIPAL RESEARCHER: ISABEL MARIA SOUSA GONÇALVES
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): -

PTDC/CTM/72093/2006 | HÍBRIDOS ORGÂNICOS-INORGÂNICOS AUTO FOTO-PADRONIZÁVEIS PARA DISPOSITIVOS DE BAIXO CUSTO EM ÓPTICA INTEGRADA
PRINCIPAL RESEARCHER: MARIA RUTE DE AMORIM E SÁ FERREIRA ANDRÉ
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 160.000,00

PTDC/CTM/73643/2006 | DESENVOLVIMENTO DE NOVOS PÓS E MEMBRANAS MICROPOROSAS
PRINCIPAL RESEARCHER: ZHI LIN
BEGINNING DATE: 01-02-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 78.000,00

PTDC/CTM/72093/2006 | HÍBRIDOS ORGÂNICOS-INORGÂNICOS AUTO FOTO-PADRONIZÁVEIS PARA DISPOSITIVOS DE BAIXO CUSTO EM ÓPTICA INTEGRADA
PRINCIPAL RESEARCHER: MARIA RUTE DE AMORIM E SÁ FERREIRA ANDRÉ
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 160.000,00

PTDC/CTM/73643/2006 | DESENVOLVIMENTO DE NOVOS PÓS E MEMBRANAS MICROPOROSAS
PRINCIPAL RESEARCHER: ZHI LIN
BEGINNING DATE: 01-02-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 78.000,00

PROGRAMA PHC-PESSOA | NEW ADVANCED HIGH-RESOLUTION SOLID-STATE NMR METHODS TO PROB 1H AND 14N NUCLEI FOR THE STUDY OF INORGANIC-ORGANIC HYBRID NANOMATERIALS
PRINCIPAL RESEARCHER: JOÃO CARLOS MATIAS CELESTINO GOMES DA ROCHA
BEGINNING DATE: 01-01-2008 | 24
FUNDING: GRICES | UA VALUE (€): 4.000,00

POCI/CTM/59425/2004 | PROCESSING AND CHARACTERIZATION OF ELECTROACTIVE POLYMERS AND COMPOSITES BASED ON PVDF FOR MICROELECTRONIC
PRINCIPAL RESEARCHER: PAULA MARIA LOUSADA SILVEIRINHA VILARINHO
BEGINNING DATE: 01-04-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 71.352,00

POCI/CTM/58312/2004 | BIOTEX - BIOACTIVE TEXTILES USING FUNCTIONAL BIOPOLYMERS
PRINCIPAL RESEARCHER: JOSÉ ANTÓNIO LOPES DA SILVA | ANDREI KHOLKIN
BEGINNING DATE: 01-07-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 33.370,00

PTDC/CTM/64805/2006 | STATICS AND DYNAMICS IF HIGHT POLARIZABLE ULTRA-THIN FILMS AND NANO-LAYERED SUPERLATTICES
PRINCIPAL RESEARCHER: PAULA MARIA LOUSADA SILVEIRINHA VILARINHO
BEGINNING DATE: 01-02-2007 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 107.505,00

PTDC/CTM/67575/2006 | PROCESSING AND CHARACTERIZATION OF MULTIFERROIC CERAMICS FOR SENSOR AND ACTUACTOR APPLICATIONS
PRINCIPAL RESEARCHER: PAULA MARIA LOUSADA SILVEIRINHA VILARINHO
BEGINNING DATE: 02-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 106.000,00

PTDC/CTM/73367/2006 | COLOSSAL PERMITTIVITY PEROVSKITE FILMS BY CHEMICAL SOLUTION DEPOSITION METHODS FOR MICROELECTRONIC AND SENSOR APPLICATIONS
PRINCIPAL RESEARCHER: AIYING WU
BEGINNING DATE: 01-03-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 85.000,00

PTDC/CTM/71643/2006 | NOVOS ÓXIDOS DE AURIVILLIUS PARA APPLICAÇÕES MICROELECTRÓNICA
PRINCIPAL RESEARCHER: MARIA ELISABETE JORGE VIEIRA COSTA
BEGINNING DATE: 01-02-2008
FUNDING: FCT | UA VALUE (€): -

POCI/CTM/61284/2004 | MATERIALS SCIENCE AND FUNDAMENTAL RESEARCH ON NANO-STRATIFIED RARE EARTH BASED COMPOUNDS FOR MAGNETIC REFRIGERATION AND SENSOR APPLICATIONS - UNUSUAL MARTENSITIC TRANSITIONS DRIVEN BY THE ELECTRONIC FLUID
PRINCIPAL RESEARCHER: VITOR BRÁS DE SEQUEIRA AMARAL
BEGINNING DATE: 01-05-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): -

POCI/CTM/60064/2004 | ELECTROPOLYMERIZED COATING USED AS PRE-TREATMENTS FOR ALUMINIUM ALLOYS
PRINCIPAL RESEARCHER: MÁRIO GUERREIRO DA SILVA FERREIRA
BEGINNING DATE: 15-07-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 17.340,00

POCI/CTM/66195/2006 | DESENVOLVIMENTO DE MICROESTRUTURAS TEXTURIZADAS E ULTRA-FINAS POR FUSÃO DE ZONA COM LASER
PRINCIPAL RESEARCHER: RUI RAMOS FERREIRA E SILVA
BEGINNING DATE: 02-01-2008 |36 MONTH
FUNDING: FCT | UA VALUE (€): 115.697,00

ANODIC FILMS ON LIGHT METALS OBTAINED BY NOVEL HIGH-VOLTAGE PULSED ANODIZING TECHNIQUE
PRINCIPAL RESEARCHER: MÁRIO GUERREIRO DA SILVA FERREIRA
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 107.202,00

PTDC/CTM/6604/2006 | SENSING THE MICRO-DISTRIBUTION OF CHEMICAL SPECIES IN SOLUTION CLOSE TO THE ACTIVE METAL
PRINCIPAL RESEARCHER: ANTÓNIO ALEXANDRE DA CUNHA BASTOS
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 82.425,00

PTDC/CTM/66302/2006 | DESENVOLVIMENTO DE UM BETÃO REFRACTÁRIO AUTO-ESCOANTE SEM CIMENTO PARA REVESTIMENTOS MONOLÍTICOS
PRINCIPAL RESEARCHER: ANA MARIA SEGADÃES
BEGINNING DATE: 07-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 139.000,00

PTDC/QUI/68472/2006 | CONTROLLED CHEMICAL MODIFICATION OF POLYSACCHARIDES FOR THE DEVELOPMENT OF NOVEL MATERIALS
PRINCIPAL RESEARCHER: CARMEN SOFIA DA ROCHA FREIRE BARROS
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 69.300,00

POCI/QUI/59337/2004 | CHARACTERIZATION OF HETEROPOLYSACCHARIDES USING MASS SPECTROMETRY
PRINCIPAL RESEARCHER: MARIA DO ROSÁRIO MARQUES | DMITRY EVTYUGIN
BEGINNING DATE: 01-10-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 64.500,00

POCI/QUI/56229/2004 | MOULD PROTEOME REGULATION BY SUBSTRATE BIOAVAILABILITY: DEPOLYMERISING ENZYMES LIKELY TO ALTER BIOPOLYMER NANOSTRUCTURE
PRINCIPAL RESEARCHER: ANA MARIA PISSARRA COELHO GIL
BEGINNING DATE: 01-06-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 19.800,00

POCI/QUI/56569/2004 | MOLECULAR RECOGNITION OF PHTHALATE AND PHTHALIC ACID ESTERS POLLUTANTS BY DITOPIC RECEPTORS OR BY CASCADE DICOPPER SYSTEMS
PRINCIPAL RESEARCHER: VITOR MANUEL SOUSA FÉLIX
BEGINNING DATE: 01-09-2005 | 36 MONTH
FUNDING: FCT | UA VALUE (€): 20.040,00

PTDC/QUI/68582/2006 | CONCEPÇÃO MOLECULAR DE NOVOS RECEPTORES DO TIPO AZACALIXARENO PARA QUÍMICA MEDICINAL: ENCAPSULAMENTO DE IÕES LANTANIDEOS E RESOLUÇÃO DE FÁRMACOS RACÉMICOS
PRINCIPAL RESEARCHER: VITOR MANUEL SOUSA FÉLIX
BEGINNING DATE: 01-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): -

PTDC/QUI/66523/2006 | ESTUDO METABONÓMICO DE DESORDENS DA GRÁVIDA E DO FETO POR ESPECTROSCOPIA DE RESSONÂNCIA MAGNÉTICA NUCLEAR (RMN): CARACTERIZAÇÃO BIOQUÍMICA E MÉTODOS DE DIAGNÓSTICO
PRINCIPAL RESEARCHER: ANA MARIA PISSARRA COELHO GIL
BEGINNING DATE: 15-01-2008 | 36 MONTH
FUNDING: FCT | UA VALUE (€): -

OTHER PROJECTS, COOPERATION AGREEMENT AND CONTRACTS | UA: COORDINATOR

BIOREFINARIA: APROVEITAMENTO DE CONDENSADOS
PRINCIPAL RESEARCHER: DMITRY VICTOROVITCH EVTYUGIN
BEGINNING DATE: 02-02-2006 | 24 MONTH
FUNDING: CAIMA | UA VALUE (€): 48.670,00

BIOREFINARIA: ELEMENTOS NÃO PROCESSUAIS NO CIRCUITO DE RECUPERAÇÃO E POTENCIALIDADES DO LICOR
PRINCIPAL RESEARCHER: DMITRY VICTOROVITCH EVTYUGIN
BEGINNING DATE: 02-02-2006 | 24 MONTH
FUNDING: CAIMA | UA VALUE (€): 48.670,00

DESENVOLVIMENTO DE NOVAS PASTAS PARA PAPEIS ESPECIAIS
PRINCIPAL RESEARCHER: DMITRY VICTOROVITCH EVTYUGIN
BEGINNING DATE: 30-06-2007 | 12 MONTH
FUNDING: PORTUCEL | UA VALUE (€): -

ESTUDO SOBRE O MELHORAMENTO DA INTERACÇÃO TINTA-PAPEL NA IMPRESSÃO OFFSET E INK-JET
PRINCIPAL RESEARCHER: DMITRY VICTOROVITCH EVTYUGIN
BEGINNING DATE: 01-07-2007 | 24 MONTH
FUNDING: RAIZ | UA VALUE (€): 25.000,00

BIOCHEMICAL CHARACTERISATION OF STOMACH, ENDOMETRIAL AND LUNG TUMOUR (HRMAS) NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY
PRINCIPAL RESEARCHER: BRIAN JAMES GOODFELLOW
BEGINNING DATE: 01-09-2006 | 36 MONTH
FUNDING: CIMAGO | VALUE (€): 9.000,00

SÍNTESE E CARACTERIZAÇÃO DE NANOMATERIAIS CERÂMICOS COM APLICAÇÕES BIOLÓGICAS E ELETROQUÍMICAS
PRINCIPAL RESEARCHER: JOSÉ MARIA DA FONTE FERREIRA
BEGINNING DATE: 01-08-2005 | 36 MONTH
FUNDING: GRICES | UA VALUE (€): -

OTHER PROJECTS, COOPERATION AGREEMENT AND CONTRACTS | UA: PARTNER

ACÇÃO Nº E-93/08, PROCº AI-E/07HIGH-RESOLUTION SOLID-STATE NMR AND POWDER DIFFRACTION TWO COMPLEMENTARY TECHNIQUES FOR THE CHARACTERIZATION OF ORGANIC-INORGANIC HYBRID NANOMATERIALS BASED ON METAL PHOSPHATES
PRINCIPAL RESEARCHER: LUÍS MIGUEL MONTEIRO MAFRA
BEGINNING DATE: 01-01-2008 | 24 MONTH
FUNDING: ACÇÃO INTEGRADA | UA VALUE (€): 4.000,00

SYNTHESIS, CHARACTERIZATION AND OPTICAL PROPERTIES OF SI, GE AND SIGE NANOCRYSTAL
PRINCIPAL RESEARCHER: NICOLA ALLESSANDRO PINNA
BEGINNING DATE: 02-01-2007 | 12 MONTH
FUNDING: GRICES | UA VALUE (€): -

MATERIAIS HÍBRIDOS ORGÂNICOS-INORGÂNICOS PARA APLICAÇÕES EM ÓPTICA INTEGRADA
PRINCIPAL RESEARCHER: LUÍS ANTÓNIO FERREIRA MARTINS DIAS CARLOS
BEGINNING DATE: 01-01-2005 | 24 MONTH
FUNDING: GRICES | UA VALUE (€): -

A NEW TECHNOLOGY FOR OBTAINING COMPLEX GLASS CHARGE FOR MANUFACTURE UVIOL GLASS
PRINCIPAL RESEARCHER: MARIA GRACINDA DA SILVA
BEGINNING DATE: 01-10-2007

PRODUCTION OF CALCIUM PHOSPHATE (CAP) NANOPARTICLES AND CAP MODIFIED SURFACES FOR CELL GUIDING AND DIFFERENTIATION STUDIES
PRINCIPAL RESEARCHER: MARIA ELISABETE JORGE VIEIRA COSTA
BEGINNING DATE: 03-04-2006 | 36 MONTH
FUNDING: GKSS | UA VALUE (€): -

CARBIFINO 70/00090 | CONCEPÇÃO DE NOVOS GRAUS DE METAL DURO DE GRANULOMETRIA SUB- A NANO-MÉTRICA COM ELEVADA RESISTÊNCIA AO DESGASTE EROSIVO
PRINCIPAL RESEARCHER: RUI RAMOS FERREIRA E SILVA
BEGINNING DATE: 02-01-2006 | 24 MONTH
FUNDING: ADI | UA VALUE (€): 74.375,00

SUB0 – AUMENTO DO TEMPO DE VIDA DE FERRAMENTAS E ORGÃOS DE MAQUINAS POR TRATAMENTO TERMICO ESPECIFICO
PRINCIPAL RESEARCHER: FILIPE OLIVEIRA
BEGINNING DATE: 01-04-2006 | 24 MONTH
FUNDING: ADI | UA VALUE (€): 21.600,00

DESENVOLVIMENTO TECNOLÓGICO APLICADO A MATÉRIAS-PRIMAS, PROCESSOS E PRODUTOS CERÂMICOS
PRINCIPAL RESEARCHER: JOÃO ANTÓNIO LABRINCHA BATISTA
BEGINNING DATE: 01-01-2005 | 48 MONTH
FUNDING: GRICES | UA VALUE (€): -

VALORIZAÇÃO DE RESÍDUOS E SUB-PRODUTOS INDUSTRIAIS NO DESENVOLVIMENTO DE MATERIAIS CERÂMICOS
PRINCIPAL RESEARCHER: ANA MARIA SEGADÃES
BEGINNING DATE: 01-05-2005 | 24 MONTH
FUNDING: GRICES | UA VALUE (€): -

APPLICATION OF NMR-BASED METABONOMICS FOR EVALUATION OF DONOR HUMAN LIVERS FOR TRANSPLANATION
PRINCIPAL RESEARCHER: ANA MARIA PISSARRA COELHO GIL
BEGINNING DATE: 01-10-2004 | 48 MONTH
FUNDING: CRUP | VALUE (€): -

DESIGN, ENGINEERING AND APPLICATION OF NANOSIZED CALCIUM PHOSPHATE PARTICLES (CAP-NP)
PRINCIPAL RESEARCHER: MARIA MARGARIDA TAVARES LOPES DE ALMEIDA
BEGINNING DATE: 03-04-2006 | 36 MONTH
FUNDING: GKSS | VALUE (€): -

A-14/07 | DESENVOLVIMENTO DE SUPORTES POROSOS PARA APLICAÇÕES
PRINCIPAL RESEARCHER: MARIA HELENA FIGUEIRA VAZ FERNANDES
BEGINNING DATE: 01-01-2007 | 48 MONTH
FUNDING: CRUP | VALUE (€): 4.500,00

Capa

Dora dos Santos | dsantos@ua.pt

Design & Lay-out

João Rocha

Dora dos Santos

SPONSORS

Portuguese Republic
Government

FCT

European Union / FEDER – European
Regional Development Fund

POCTI Programa Operacional Ciência Tecnologia Inovação

Ciência.Inovação
2010

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