



RELATÓRIO DE

ACTIVIDADES

2003

e

PLANO DE ACTIVIDADES

2004

Índice dos Documentos

	Nº de páginas
Summary of Year 2003 key Features and Activities	3
Relatório de Actividades 2003	17
Produção Científica	78
Outras Actividades	4
Projectos	8
Plano de Actividades 2004	14

SUMMARY OF YEAR 2003 KEY FEATURES AND ACTIVITIES

1) Research Team

On December 2003, CICECO comprised 206 people:

- 47 University Professors and Lecturers
- 9 Full time researchers
- 3 Administrative personnel
- 8 Laboratory technicians
- 22 post-doctoral associates
- 60 Ph.D. students
- 44 others students (M.Sc., BIC...)
- 13 other scientists from National institutions were also considered as CICECO direct collaborators.

2) Scientific Output

Ph. D. Thesis Finished	13
M.Sc. Thesis Finished	8
SCI Papers	224
Non SCI Papers and Proceedings of International Conferences (≥ 4 pages)	77
Book Chapters (international publishers)	5
Book Chapters (national publishers)	9
National Patents	3
Short Abstracts in Conference Books	196

On December 2003, 100 financed projects were in progress. One EU Network of Excellence (“Advanced Materials Engineering of Hybrids and Ceramics”) and one IP (“Innovation and Sustainable Development in the Fibre Based Packaging Value Chain”) were approved, together with the INTERREG III “Materials Network for the Atlantic Area”. Our Marie Curie training Centre, (HPMT-CT-2000-00206) Advanced Ceramics-Synthesis and Structure, received 2 PhD Students.

3) Management and Organisation

a) As far as strategic management of CICECO is concern, Prof. Paulo Vilarinho and his team, in collaboration with the extended Direction Board, carried out a major

exercise using the so-called “Balance Score Card” model. A paper is in preparation presenting the results of this work.

b) Current management activities in 2003 included:

- About 1500 financial documents processed.
- Monthly updates on the current financial situation of each senior researcher.
- Considerable increase in the number of projects now managed by CICECO’s administrative people.
- Improvement of the system used for gathering relevant information and data on the scientific production of CICECO’s researchers.
- Monthly meetings of the extended Direction Board.
- Production of the 2002 Report and the 2003 Financial Plan
- Determination of the number of “personal credits” of each senior researcher and the resultant financial grant.

c) A considerable effort has been put into ensuring that all CICECO’s equipment is now fully operational and available to all our researchers and graduate students. In addition, the laboratory in “Laboratório Central de Análises” is now fully set up, after major work particularly in the gas exhaust system.

d) Three new full-time researchers have been contracted: Dr. Zhi Lin, Rute André (area 1) and Filipe Oliveira (area 2). In addition, Dr. Paula Brandão has been contracted as a technician (at present in charge of solid state NMR, later she will be involved with single crystal XRD) and Carla Ranito as the third administrative person of CICECO.

e) External activities in 2003 included:

- Monthly meetings of CICECO’s Directors with the “Associated Laboratories Council” (one of the meetings took place in Aveiro), contributing to the production of Science and Technology policy papers.
- Meetings with people having political responsibilities in the areas of Science and Technology, particularly the Portuguese President, the Minister of Science and Universities, the President of the National Science Foundation (FTC).

4) “Centre for the Design and Technology of Materials” (CDTM)

- The Directing Board of CDTM now includes Profs. António Fonseca (Director) and João Labrincha (Vice-Director).
- The strategy of CDTM has been clarified; the financial situation has been improved considerably as a result of a successful project submitted (see below).

In 2003, the CDTM developed several activities:

- Publicising the centre to all regional and national companies. One awareness seminar has been carried out, entitled: “Opportunities of participation in the 6^o Framework Programme of research and Technological Development”; the majority of participants came from local companies. A short course, entitled “Technology Commercialisation” has been organised in collaboration with Prof. Angus Kingon (Carolina State University, USA); participants (scientists and industrialists) discussed the best practices of technology transfer and commercialisation.

-
- Applied R&D activities. Two new contracts were established with national companies, in which CTDM provides technological support. Three other contracts are under discussion.
 - Identification of potential funding sources for join Industry/Academic research programmes. The CDTM successfully applied for funding in the framework of the EU programme INTERREG IIIB with other EU countries: UK, Ireland, France and Spain. This project aims at deeper, lasting, formal integration between partners to create an internationally recognised centre of expertise in Materials, the “Materials Network for the Atlantic Area”, and also a broader connection to steadily widening sub-networks of start-ups, SMEs and larger industrial concerns. This project starts on 1st January 2004.

RELATÓRIO

DE

ACTIVIDADES

2003

AREA 1

ADVANCED MICRO- AND NANO-STRUCTURE MATERIALS FOR COMMUNICATIONS TECHNOLOGIES

Inorganic Multifunctional Materials and Organic-Inorganic Hybrids

New Microporous Materials. The main achievement in 2003 in this area was the synthesis and characterisation of structure and photoluminescence (PL) of microporous lanthanide silicates in the system $(\text{Na}_{1.08}\text{K}_{0.5}\text{Ln}_{1.14}\text{Si}_3\text{O}_{8.5}\cdot 1.78\text{H}_2\text{O})$, Ln=Eu, Tb, Sm, Ce). The structure of these materials is closely related with the structure of hydrated calcium silicate minerals known as tobermorites. They combine microporosity with efficient PL, tunable by introducing a second type of Ln ion in the framework. Thus, they may find applications in new types of sensors. The synthesis by sol-gel methods of (dense) titanosilicate narsarsukite, and the characterisation of PL properties has also been reported. Another milestone of the year was the synthesis of the small pore material AV-13 $(\text{Na}_{2.26}\text{SnSi}_3\text{O}_9\text{Cl}_{0.26}\cdot x\text{H}_2\text{O})$ and zirconium and hafnium analogues of this material whose structure has been solved from powder XRD data using direct methods, and solid-state NMR. To describe adequately the structure the new concept of three-dimensional knots-and-crosses lattice has been introduced. Two novel large-pore vanadium silicate redox catalysts (AM-15 and AM-17) and two novel (dense) tin and titanium potassium silicates (AV-11 materials) have been reported. As a final milestone of 2003, combination of advanced powder diffraction (synchrotron data and programme FOCUS) and NMR techniques allowed the structure of the novel and unusual microporous aluminophosphate IST-1 to be. The crystal structure of microporous hybrid $(\text{CH}_3\text{H}_{12}\text{N}_2)[\text{V}_3\text{O}_3(\text{OH})_2(\text{PO}_4)_2]\cdot 2\text{H}_2\text{O}$ has been redetermined with improved precision from single-crystal X-ray data recorded at 180 K. Two pieces of work on 'conventional' zeolites have been published: (i) the nitrate occlusion in zeolite Y (with some unexpected ^{15}N MAS NMR evidence); and (ii) the oxidation of monoterpenes catalysed by a Mn(III)-porphyrin complex entrapped on zeolite Y. Finally, membranes and films of titanosilicate ETS-10 supported on alumina and stainless steel have been prepared and a paper submitted for publication.

Mesoporous Materials. Purely siliceous mesoporous materials functionalised with oxomolybdenum complexes were prepared by primary (direct grafting) or secondary (tethering) methods. (i) Primary grafting. Mo K-edge X-ray absorption spectra were measured at the ESRF for MCM-41 grafted with the complexes $\text{MoO}_2\text{X}_2(\text{THF})_2$ (X = Cl, Br). For reactions carried out in the absence of triethylamine, materials with 1 wt.% Mo were obtained and the EXAFS results indicated the existence of isolated surface-fixed monomeric species of the type $\{\text{MoO}_2[(-\text{O})_3\text{SiO}]_x\text{X}_{2-x}(\text{THF})_n\}$ (x = 1,2). The EXAFS data for the material prepared using $\text{MoO}_2\text{Cl}_2(\text{THF})_2$ and Et_3N (4 wt.% Mo) indicated the presence of dinuclear species with two Mo^{VI} centres, each with two Mo=O groups and both linked by one or two oxo bridges ($\text{Mo}\cdots\text{Mo} = 3.27 \text{ \AA}$). These materials were used as catalysts for the liquid-phase oxidation of olefins and alcohols. (ii) Tethering. The dioxomolybdenum(vi) complexes $\text{MoO}_2\text{Cl}_2(\text{L-L})$, containing the 1,4-diazabutadiene ligands $\text{RN}=\text{C}(\text{Ph})-\text{C}(\text{Ph})=\text{NR}$ [R = $(\text{CH}_2)_3\text{Si}(\text{OR}')_3$, R' = Me or Et), were immobilised in MCM-41 and MCM-48 by covalent bonding. Tethered complexes of this type were also prepared by an alternative stepwise approach. The modified materials were characterised by powder XRD, N_2 -adsorption and $^{13}\text{C}/^{29}\text{Si}$ MAS NMR, and tested as olefin epoxidation catalysts using *tert*-butyl hydroperoxide.

Benzene-silica hybrid materials exhibiting meso- and molecular-scale periodicity were prepared using surfactant templates with different alkyl-chain lengths. The resulting quasi-crystalline materials possess similar lattices but different pore sizes (3.2–3.9 nm). The benzene groups are preserved in the walls up to 550 °C for all samples.

Layered Materials. The acceptable levels of sulphur in liquid hydrocarbon fuels are continually on the decrease. To eliminate undesirable sulfur compounds (e.g., thiophenes) or to convert them into more innocuous forms, various non-conventional processes have been employed or are being investigated, such as oxidative desulphurisation. We discovered that the polymeric organotin-oxomolybdates $[(\text{R}_3\text{Sn})_2\text{MoO}_4]\cdot n\text{H}_2\text{O}$ (R = methyl, *n*-butyl, cyclohexyl, phenyl, benzyl) are effective catalysts for the sulfoxidation of benzothiophene with H_2O_2 , at 35 °C and atmospheric pressure. The liquid oxidation process produces sulfones (can be used as surfactants) that can be physically separated and downstream processed. Catalytic results depend on the complex interplay between various factors, such as the addition of co-solvents and the hydrophobic/hydrophilic properties of the starting polymers. Changing the nature and size of the tin-bonded R groups influences catalytic performance, by inducing structural

changes and modifying the surface polarity/polarisability of the compounds. Mo *K*-edge and Sn *K*-edge EXAFS studies on these coordination polymers confirmed that the structures arise from the self-assembly of tetrahedral $[\text{MoO}_4]^{2-}$ anionic sub-units and $[\text{R}_3\text{Sn}]^+$ cationic spacers. The Mo...Sn separation in the trimethyltin derivative is a uniform 3.84 Å. By contrast, the EXAFS results reveal the coexistence of short (3.67–3.79 Å) and long (3.93–4.07 Å) Mo...Sn separations in the other coordination polymers.

Layered double hydroxides (LDHs), have been prepared and characterized by FTIR, FT Raman, ^{13}C MAS NMR and TGA. Ferrocenecarboxylates have been intercalated and the resulting materials investigated.

Nanostructured Materials. Bi_2S_3 nanofibers have been coated with SiO_2 using the alkaline hydrolysis of $\text{Si}(\text{OEt})_4$. A comparative study on the optical and morphological properties of the starting Bi_2S_3 nanofibres and the final SiO_2 -coated nanomaterials was carried out. A SiO_2 cap covering homogeneously single Bi_2S_3 nanofibres was obtained when the hydrolysis of $\text{Si}(\text{OEt})_4$ was performed under sonication to maintain the fibres well separated during the coating process. These coated nanofibers were then used in a layer-by-layer deposition process to produce multilayered nanostructured films.

Complexes $[\text{Bi}\{\text{Se}_2\text{CN}(\text{C}_2\text{H}_5)_2\}_3]$, $[\text{Bi}\{\text{Se}_2\text{CN}(\text{C}_4\text{H}_9)_2\}_3]$, $[\text{Bi}\{\text{Se}_2\text{CN}(\text{CH}_3)(\text{C}_4\text{H}_9)\}_3]$ and $\text{Bi}\{\text{Se}_2\text{CN}(\text{CH}_3)(\text{C}_6\text{H}_{13})\}_3]$ have been synthesised and characterised structurally by IR, and ^{13}C NMR. In addition, the crystal structure of $[\text{Bi}\{\text{Se}_2\text{CN}(\text{C}_4\text{H}_9)_2\}_3]$ was determined by single-crystal X-ray diffraction, showing the bismuth centre coordinated to three dialkyldiselenocarbamate ligands through the selenium donor atoms. The Bi(III) compounds were used as precursors for the deposition of Bi_2Se_3 films on glass substrates through aerosol-assisted metallo-organic chemical vapour deposition (AA-MOCVD).

Novel Pigments. The preparation of Ce doped BiVO_4 coatings on glass, by the thermal treatment of aqueous solutions containing a bismuth (III)ethylenediaminetetra-acetate chelate vanadium (V) and cerium (III) species, was performed. The influence of the cerium content on the colour properties of the coating was investigated. The coatings consist on morphological well-defined particles forming dense monolayers.

The encapsulation of hollow-ZnO microparticles with the BiVO_4 pigment was performed. The crystalline phases present in the composite ZnO/BiVO_4 microparticles were investigated by X-ray powder diffraction (XRD) studies and Raman spectroscopy. The micrometric ZnO/BiVO_4 particles show morphological characteristics related to the hollow-ZnO particles used as templates.

Polyoxometallates. New compounds with general formula $(\text{MeLeu})_y[\text{XW}_{11}\text{Mn}(\text{H}_2\text{O})]\cdot x\text{H}_2\text{O}$, X = P, Si, B, (y depending on the anion charge) and $(\text{Me}_2\text{Asp})_y[\text{XW}_{11}\text{Mn}(\text{H}_2\text{O})]\cdot x\text{H}_2\text{O}$, X = P, B, where MeLeu and Me₂Asp are protonated L-leucine methyl ester and L-aspartic dimethyl ester, respectively, were prepared and characterised (TGA, FTIR, UV/Vis). These compounds were used in catalytic studies of oxidation of cyclooctane and geraniol with hydrogen peroxide. Catalytic studies of oxidation of cicloalkanes and ethylbenzene with H_2O_2 , in acetonitrile, in the presence of Keggin and sandwich type anions were continued.

Tetra-n-butylammonium salts of several Keggin-type transition metal-substituted polyoxotungstates were immobilised in carbon electrodes and their electrochemical properties studied by cyclic voltammetry. Some of the immobilised polyoxoanions were tested as electrocatalysts.

Electrochemical studies of copper substituted anions $[\text{PW}_{11}\text{CuO}_{39}]^{5-}$ and $[\text{Cu}_4(\text{PW}_9\text{O}_{34})_2(\text{H}_2\text{O})_2]^{10-}$ in acetonitrile were performed. An unusual two-step reduction of Cu(II) to Cu(0) with the formation of intermediate species containing Cu(I) was detected. The fact that this behaviour was never observed before in studies in aqueous solutions was attributed to the influence of acetonitrile in the stabilisation of Cu(I). The intermediate reduction to Cu(I) was also observed during reduction of the anion α - $[\text{PW}_{11}\text{CuO}_{39}]^{5-}$ immobilised on the surface of a glassy carbon electrode in the form of adsorbed tetrabutylammonium salt.

Characterisation of the compounds $[\text{O}_2\text{N}(\text{C}_6\text{H}_5\text{N})\text{NH}_2]_x\text{H}_y[\text{XM}_{12}\text{O}_{40}]\cdot n\text{ solv}$, (X = P, Si, M = Mo, W) was completed. Some of the compounds could be prepared in two differently coloured forms. Studies of their nonlinear optical properties are in progress. In line with these studies, new compounds with the same anions and urea and tetramethylurea were prepared and are being characterised.

New lanthanopolyoxotungstoborates $\text{K}_{6-x}\text{H}_x[\text{Ln}(\text{BW}_{11}\text{O}_{39})(\text{H}_2\text{O})_3]\cdot n\text{H}_2\text{O}$, Ln(III) = Sm, Eu, Tb, Er, were prepared and characterised (FTIR, FT-Raman, ^{11}B solid state NMR and photoluminescence). A layer-by-layer assembly method was used to fabricate multi-layered films containing the europium heteropolyanion and polyelectrolytes. The photoluminescence behaviour of these final nanostructures

was investigated. A new polyoxotungstoeuropate was prepared and encapsulated with high molecular weight cations. Photoluminescence studies were performed on monolayers transferred to a quartz substrate using the Langmuir-Blodgett technique.

Novel Luminescent Systems. The synthesis, luminescence properties, experimental determination and theoretical calculation of the emission quantum yield of $\text{Eu}(\text{NTA})_3 \cdot 2\text{L}$ (NTA = naphthyltrifluoroacetone; L = H_2O , dimethyl sulfoxide, DMSO), complexes were reported. The quantum yield measured, 0.75, is one of the highest reported so far for solid-state Eu^{3+} complexes and agrees with theoretical calculations of the quantum yield. The photostability of $\text{Eu}(\text{NTA})_3 \cdot 2\text{DMSO}$ at 358 K was evaluated in order to evaluate the potential of this complex for application in blue light emitting devices. Some of the basic aspects of rare-earth spectroscopy applied to vitreous materials were reviewed. The characteristics of the intra-atomic free ion and ligand field interactions and the formalism of the forced electric dipole and dynamic coupling mechanisms of 4f–4f intensities, were outlined. The contribution of the later to the 4f–4f intensities was critically discussed, an issue overlooked in the literature. The observed correlation between the empirical intensity parameter Ω_2 and the covalence of the ion first coordination shell was discussed accordingly to the theoretical predictions.

Research was carried out on the synthesis of photoactive lanthanide complexes. The possibility of the ligands to function as remote light-harvesting units, acting as an antenna for collecting light and transferring the energy to the lanthanide, was particularly investigated. Research was done on the coordination of lanthanides by derivatised fullerenes and aromatic ambidentate ligands. New complexes of 2-hydroxynicotinic acid (H_2nicO) [$\text{Ln}(\text{HnicO})_2(\mu\text{-HnicO})(\text{H}_2\text{O})$] $\cdot n\text{H}_2\text{O}$ (Ln = Eu, Gd, Tb, Er, Tm) were prepared and the crystal structures of the Tb and Eu complexes determined. nicO ligand coordinates via *O,O*-chelation to the Ln(III) ions, as shown by powder XRD, FTIR, Raman and NMR. Photoluminescence measurements were performed for the Eu(III) and Tb(III) complexes. The Er(III) complex of picolinic acid (Hpic), [${}^{\text{t}}\text{Bu}_4\text{N}$][$\text{Er}(\text{pic})_4$] $\cdot 5.5\text{H}_2\text{O}$ (an infrared emitter), was synthesised and the crystal structure determined. Lanthanide complexes of 2,6-dihydroxybenzoic acid (2,6-Hdhhb), namely [${}^{\text{t}}\text{Bu}_4\text{N}$] $[\text{Ln}(2,6\text{-dhb})_3(\text{H}_2\text{O})_2]$ (Ln = Sm, Tb), were synthesised and their structures determined by single-crystal XRD. The 2,6-dhb ligand coordinates the Ln cations through the carboxylate group in a monodentate or bidentate mode. The terbium complex shows intense photoluminescence in the solid state and in ethanolic solution, and is triboluminescent. New complexes of 3-hydroxypicolinic acid (HpicOH) were prepared: [$\text{Ln}(\text{H}_2\text{O})\text{-}(\text{picOH})_2(\text{HpicO})$] $\cdot 3\text{H}_2\text{O}$ (Ln = Eu, Tb, Er) and characterised. The crystal structure of [$\text{Eu}(\text{H}_2\text{O})(\text{picOH})_2(\text{HpicO})$] $\cdot 3\text{H}_2\text{O}$ was determined by XRD. The 3-hydroxypicolinate ligands coordinate the Ln ions through *N,O*- and *O,O*- chelation. The Eu(III) compound is strongly luminescent and acts as a photoactive centre in nanocomposite materials whose host matrixes are silica nanoparticles.

One of the main achievements in 2003 in this area was the synthesis and characterisation of structure and photoluminescence (PL) of lanthanide silicates $\text{Na}_3(\text{Y}_{1-a}\text{M}_a)\text{Si}_3\text{O}_9$ (M = Tm^{3+} , Tb^{3+} ; a=0-1), isostructural with $\text{Na}_3\text{YSi}_3\text{O}_9$. The Tm-based materials display quite unusual room-temperature (RT) luminescence features in the blue and infrared regions. While $\text{Na}_3\text{TmSi}_3\text{O}_9$ shows a broad RT emission within the *E* (Extended), *S* and *C* bands (ca. 1360-1565 nm), which is essential for the new generation of silica-based TDFA, $\text{Na}_3(\text{Y}_{1-a}\text{Tm}_a)\text{Si}_3\text{O}_9$ displays a blue emission with (x,y) CIE (Commission Internationale de L'Eclairage) colour coordinates and colour purity comparable to, or better than, those reported for the mostly used blue phosphors. Tuning of the infrared emission between the *S* and the *O* (Original) bands is easily achieved by controlling the $\text{Y}^{3+}/\text{Tm}^{3+}$ molar ratio. Moreover, $\text{Na}_3(\text{Y}_{1-a}\text{Tb}_a)\text{Si}_3\text{O}_9$ terbium-based sodium silicates are new and highly efficient X-ray phosphors with potential applications in medical diagnostic imaging systems (ca. 25% brighter than $\text{Gd}_2\text{O}_2\text{S:Tb}$).

New Hybrid Materials. The photoluminescence features and energy transfer processes of Nd^{3+} -based diureasils were reported. The room-temperature photoluminescence spectra of these xerogels show a wide broad purple-blue-green band (350-570 nm) associated with the emitting centres of the di-ureasil host, and the typical near-infrared emission of Nd^{3+} (700-1400 nm) assigned to the ${}^4\text{F}_{3/2} \rightarrow {}^4\text{I}_{9/2,11/2,13/2}$ intra- 4f^3 transitions. Self-absorptions in the visible range, resonant with intra- 4f^3 transitions, indicate the existence of an energy conversion mechanism of visible di-ureasil emission into near infrared Nd^{3+} luminescence, whose efficiency changes with the polymer molecular weight and Nd^{3+} concentration. Eu^{3+} - β -diketone complexes, such as $\text{Eu}(\text{thenoyltrifluoroacetone})_3(\text{H}_2\text{O})_2$, were incorporated into the di-ureasil host. The quantum efficiency calculated from the decay of ${}^5\text{D}_0$ emission (74%) is in the range observed for the most efficient Eu^{3+} coordination compounds. Luminescence, X-ray absorption and infrared absorption data lead to a picture where the first coordination shell of Eu^{3+} is composed of the 6 β -diketonate oxygen atoms and 2 ether-like host oxygens.

In contrast to precipitation techniques, sol-gel is suitable method to achieve the controllable formation of nanoscopic magnetic aggregates. The formation of ferrihydrite ($\text{FeOOH}\cdot n\text{H}_2\text{O}$) nanoparticles in iron-doped di-ureasils and their structural and magnetic characterisation were discussed. SAXS and FTIR studies show that the Fe(II) ions interact mainly with the organic chain, whereas the incorporation of Fe(III) into the hybrid leads to the formation of iron-based nano-clusters, with radius increasing from 20 to 40 Å. Fe(II)-doped samples behaved as simple paramagnets, with $\mu_{\text{eff}}=5.32\mu_{\text{B}}$, residual antiferromagnetic interactions ($T_{\text{N}}<2\text{K}$ up to 6% doping) and negligible zero-field vs. field-cooling thermal irreversibility. Fe(III)-doped hybrids presented a much more interesting behaviour. The high temperature susceptibility revealed antiferromagnetic interactions, with T_{N} increasing with Fe(III) concentration up to 13.6K for 6% doping. Thermal magnetic irreversibility was observed below about 40 K and is stronger for higher concentrations. The coercive fields (H_{C}) were of the order of 1000 Oe at 5 K. The hysteresis cycles are shifted to negative fields, revealing the presence of exchange anisotropy interactions. The exchange fields (H_{E}) are of the order of a few hundred Oe. Both characteristic fields decrease rapidly with increasing temperature. This behaviour, analogous to protein ferritin, unlike ferrihydrite powder systems, was analysed in terms of the contribution of surface spin disorder to exchange anisotropy, as found in nanoparticle systems of maghemite or ferrites. In order to have a better understanding of the particle aggregation mechanism occurring in these iron-doped hybrids and optimising their magnetic properties, the structural evolution during sol formation, sol-gel transition and gel aging has been investigated by SAXS. The experimental SAXS curves, corresponding to sols and gels, exhibit features that strongly depend on the nature of the iron species (Fe^{2+} or Fe^{3+}). For hybrids doped with Fe^{2+} , the sol is constituted of particles of nanometric size without spatial correlation between them and diluted in the solvent. This structure does not suffer important changes during the gelation process. SAXS patterns of Fe^{3+} -doped composites are quite different showing the existence of a two-level hierarchical structure. The first level is constituted by particles of nanometric size and the second level by large aggregates probably formed by the segregation of particles that constitute the first level. The number and the size of the aggregates are modified during the gelation process.

C60 Phase Transitions Under High Pressure. The study of polymeric phase transitions of C60 under high-pressure and high-temperature by XRD was continued. Polymerised C60 is a frustrated system and the uniaxial component of stress permits the system to escape frustration leading to ordered structures. The behaviour of C60 above 8 Gpa was studied by *in situ* XRD: novel 3D polymeric structures were found and their structural determination is under way.

Development of Spectroscopic Techniques. The double-resonance decoupling for resolution enhancement of ^{31}P solid-state MAS and $^{27}\text{Al}\rightarrow^{31}\text{P}$ MQ-HETCOR NMR has been reported but appeared (for editorial reasons) still in 2002. Two papers have been published which are considered milestones in the study of half-integer quadrupolar nuclei in solids: (i) the first one introduces a new high-resolution method, named Inverse Satellite Transition Magic-Angle Spinning (I-STMAS); (ii) the second paper assesses the potential of fast amplitude modulation pulses (FAM) for getting better triple-quantum MAS spectra and introduces some improvements in this method.

The interaction of aromatic O, S and N donor ligands with metal nanoparticles was studied by Surface Enhanced Raman Scattering (SERS), particularly the adsorption modes and orientation of molecules on the surfaces, with relevance in heterogeneous catalysis and nanoparticle assembly. A detailed vibrational study on the isomers 2,2'-dithiodipyridine and 4,4'-dithiodipyridine was carried out. Because these ligands are of great interest as possible linkers in the fabrication of nanostructures, a study on the adsorption modes of both ligands at silver surfaces was performed. Orientation information on the 2,2'-dithiodipyridine and 4,4'-dithiodipyridine molecules adsorbed on silver colloids was collected based on the SERS spectra and supported by *ab initio* calculations.

Electroceramics

Microwave Ceramic Dielectrics. New solid solutions with LMT were developed based on LT ($\text{La}_{2/3}\text{TiO}_3$) and NMT ($\text{Nd}(\text{Mg}_{1/2}\text{Ti}_{1/2})\text{O}_3$) and its processing conditions were optimised to yield single phase dense ceramics. Regarding LMT-NMT solid solutions, no significant structure transformations were observed. Permittivity and τ_f were measured in the GHz range and analysed with respect to composition (x). Non-monotonic dependence of Q on x was described according to the damped classical oscillator model and assuming two-mode behaviour of the A-BO₆ vibration mode. The LMT-LT solid solutions are very interesting and they exist as such until $x\leq 0.5$. Close to zero, τ_f exists near to

$x=0.5$ at interesting values of ϵ_r (45) and $Q \cdot f_0$ (10000). Structure transformations were related to the variation of dielectric properties.

Solid solutions of LMT with CaTiO_3 , SrTiO_3 and BaTiO_3 , previously processed by a chemical route as nanopowders, were obtained as dense, single-phase ceramics in all the range ($0 \leq x \leq 1$). Far infrared spectroscopy of all these compositions was continued and covered all the solid solution range. Extrapolations from the far infrared region down to the microwave range allowed the study of factors controlling the microwave properties. Processing, structure and dielectric properties of these systems were reported.

Microwave losses, also assessed by far infrared spectroscopy, are essentially intrinsic and for the case of LMT-BT an additional mechanism based on ionic conduction is present at rich BT compositions. A singular relaxor behaviour was detected for $x > 0.9$, which is interesting because this is a non-lead material.

Ordered $\text{Ba}(\text{M}_{1/2}\text{W}_{1/2})\text{O}_3$ ($\text{M} = \text{Mg}, \text{Zn}, \text{Ni}$) perovskites were obtained by normal ceramic processing at 1200°C . Electronic hopping between Ni and W, even at room temperature, makes dielectric losses very high and the material not suitable for microwave applications. In contrast, Mg and Zn-based materials present low losses. In these two cases, the temperature coefficient of permittivity is positive and this was explained by a considerable influence of the second polar mode of vibration, involving the B-site ion, on the low-frequency dielectric response.

Ferroelectric Ceramics. The crystalline structure of the solid solution $(1-x)\text{Pb}(\text{Fe}_{2/3}\text{W}_{1/3})\text{O}_3-x\text{PbTiO}_3$ (PFW-PT) with $x=0, 0.2, 0.25, 0.3, 0.35, 0.4$ and 1 was analysed using X-ray diffraction (XRD) with comparative cell-refinement methods, in order to detect the change in symmetry with composition and temperature. Pure PFW shows pseudo-cubic symmetry for temperatures in the range 85–423 K. At $T=85$ and 300 K, the solid solutions have cubic or tetragonal structures. The cell constants are functions of PbTiO_3 amount. A temperature-dependent Morphotropic Phase Boundary separating the pseudo-cubic (relaxor) and tetragonal (ferroelectric) phases may be present. The ranges of compositions for this boundary are: $x < 0.2$ at $T=85$ K and $x = (0.3, 0.35)$ for $T=300$ K.

The low-field dielectric response of PFW-PT ceramics with various x , was studied. The permittivity data were analysed with empirical laws describing the diffuse phase transitions in relaxors. A change of the character of the phase transition was found with increasing x , from a total diffuse, characteristic of relaxors, to a sharp one, typical of ferroelectrics. The deviations from the Curie-Weiss law of the dielectric constant data in the paraelectric phase were used to calculate a local order parameter within a modified-Landau theory for relaxors. The nonzero values of the local order parameter far above the Curie region indicate the thermal stability of the polar nanoregions in the relaxor state. The temperature dependence of the local order parameter clearly shows the evolution of the system from a short range ordered to a long range ordered ferroelectric, with increasing the PbTiO_3 addition.

A new methodology to stabilise the perovskite phase in $(1-x)\text{Pb}(\text{Zn}_{1/3}\text{Ta}_{2/3})\text{O}_3-x\text{PbTiO}_3$ [(1-x)PZTa-xPT] ($x=0.00-0.80$) ceramics was used. This approach combines the maximisation of the crystal-chemical and thermodynamics requirements and the optimisation of the kinetics of the perovskite phase formation by using highly reactive PT nucleus. For comparison, PZTa-PT ceramics were prepared through a conventional mixed oxide procedure (Columbite method). The effect of PT seeds was evaluated on the formation of the perovskite phase, microstructure and dielectric properties. The analysis of the phase formation process by DTA and XRD showed that PT seeds promote the perovskite formation in the $\text{Pb}(\text{Zn}_{1/3}\text{Ta}_{2/3})\text{O}_3$ system at lower temperature and content. Pure perovskite was obtained at $x=0.60$ by the PT seeds method and at $x=0.75$ by the mixed oxide method. The dielectric permittivity of 0.40PZTa-0.60PT ceramics prepared by the PT seeds method is 13800, at 1 kHz, which compares with 5800 at 1 kHz for the oxide mixture sample. These results demonstrate that the reaction with nanometric PT seeds is effective to promote the stabilisation of the perovskite phase in the PZTa system at low temperatures and at a low PT concentration and to improve the microstructure, that allows a maximisation of the dielectric properties of these ceramics.

Nanoscale Properties of Ferroelectrics. The local electromechanical properties of ferroelectric thin films (PZT, PMN-PT, $\text{PbTiO}_3:\text{Ca}$) and bulk ceramics (PZT, PMN-PT) were investigated by Scanning Force Microscopy (SFM). The piezoelectric properties of doped PbTiO_3 films were found to be extremely sensitive to a small force applied to the SFM tip. The piezoelectric coefficient could be suppressed almost to zero and even change the sign for one type of domains. The piezoelectric hysteresis loops acquired under increasing force were found to shrink with an asymmetric decrease of the piezoelectric coefficients. This leads to a pronounced vertical shift, and polarization offset. The results were explained based on the phenomenological theory predicting phase transition under the high

stress (~10 GPa) exerted by the tip. Thus, SFM may be used as a nanopatterning tool in ferroelectric materials using only mechanical variables (stress, strain).

Another important result concerns the piezoelectric properties of $\text{PbZr}_{0.55}\text{Ti}_{0.45}\text{O}_3$ thin films. Analysis of a SFM signal revealed that as-grown films possess high self-polarization caused by the internal bias field near the surface. The written domains with polarization oriented opposite to the self-polarization direction are unstable and rapidly switch back with time. The dynamics of the back-switching process depends strongly on the films microstructure and is slower in the regions with higher density of grain boundaries. Thus, the grain boundaries in polycrystalline ferroelectrics serve as pinning centres preventing domain wall displacement.

High-quality single crystals of ferroelectric relaxors on the system $(1-x)\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3-x\text{PbTiO}_3$ were obtained from the Department of Physics of Rostov State University (Russia). The compositions with $x=0.1$ and 0.2 are isotropic on the macroscopic scale and we have clearly observed nanoscale domains with a broad distribution of sizes (down to 10 nm). We suggest that these domains represent remnants or agglomerates of the polar clusters, the units responsible for the remarkable dielectric and piezoelectric properties of relaxors. The distribution and dynamics of these clusters were investigated.

The local electromechanical properties of single crystals of $\text{PbZn}_{1/3}\text{Nb}_{2/3}\text{O}_3-0.045\text{PbTiO}_3$ having giant piezoelectric effect (piezocoefficient over 2500 pm/V) were studied [crystal orientations (001) and (111)]. Irregular domain patterns with sizes 20-100 nm were observed in (001)-oriented samples. In contrast, (111) crystals exhibited normal micron-size regular domains with the domain boundaries directed along allowed crystallographic planes. The nanodomains in (001) crystals were considered as the nuclei of the opposite polarization state and are responsible for the smaller coercive field and giant piezoelectric effect exhibited by these crystals. Local piezoelectric hysteresis performed by SFM on the nanometer scale showed a similar switching behaviour for both orientations and local rhombohedral-to-tetragonal phase transition was not observed in (001) crystals. Thus, local electromechanical properties are very different from the macroscopic properties and may be used for identifying the intrinsic or extrinsic nature of the high piezoelectric performance.

Next, we have studied the domain structure of PZT ceramic samples with composition on the tetragonal side of morphotropic phase boundary at the different fatigue stages and compared it with the domain structure in virgin samples and in samples annealed after fatigue tests. We found that in virgin samples the so-called “watermark” contrast (180° domains) occupy the major part of the sample surface. Ferroelastic domains are occasionally observed in the vicinity of the macroscopic defects, where essential mechanical stresses are expected. After fatigue we found that the relative area occupied by ferroelastic domains grew significantly. The observed decrease of the mean domain size is a consequence of this fact. After annealing, the initial relation between 180° and ferroelastic domains was restored along with restitution of switchable polarization. The anisotropy of the domain structure changes relative to fatigue direction was investigated in detail. The fatigue effect is stronger in the plane parallel to fatigue direction than in the surface perpendicular to it. The results are essential for the understanding of the nature of fatigue in bulk ceramics.

Ferroelectric Fibres, Single Crystals and Films. PZT fibres were prepared by the sol-gel method. Different organic and inorganic acids were used to change the pH value of PZT precursor. The chemical modification of the solutions, crystallisation behaviour, microstructure and handling strength of the PZT fibres obtained from the modified solutions was compared. Using acetic and methacrylic acids to adjust the solution pH, hydrolysis and condensation changed and the macroscopic properties of PZT gel fibre improved after heat treatment. Longer PZT fibres, about 43 μm in diameter and 4-5cm long, were prepared when methacrylic acid was used. FTIR indicates that the C=C bond in the methacrylic acid solution attracted more bonds to join together in a longer molecular linear chain structure in PZT gel and, consequently, longer fibers may be pulled. Thermal and XRD analysis showed that the chemical structure modification of the precursors altered the thermal behaviour of the fibres. Longer polymeric chains were formed in the PZT precursor, and the perovskite phase was formed around 350 $^\circ\text{C}$. Single perovskite phase was obtained after the fibres were heat-treated at 550 $^\circ\text{C}$. Using acetic acid to control the precursor hydrolysis, dense and homogeneous PZT fibres were obtained, but they were shorter than the previous ones. Pure perovskite phase was formed at 700 $^\circ\text{C}$. PZT (52/48) fibres were also prepared using precursor solutions acidified with a mixture of acetic acid and methacrylic acid. The acid ratio ($\text{CH}_3\text{COOH}/\text{C}_4\text{H}_6\text{O}_2$) markedly affects the fibres macroscopic properties (length and strength) and reflects the effect of each individual acid. As the acetic acid content increases, round and crack-free fibres were obtained. As the methacrylic acid content increases, longer and cracked fibers were prepared. The molecular structure of the solution precursors, the phase formation processes and the microstructure of the fibers also depend on the ratio of the acid mixture. As the content of methacrylic acid increases, longer polymeric chains are formed in the precursor, which resulted in longer gel and

ceramic fibers and also in a low formation temperature of the perovskite phase. The length and handling strength of PZT fibres prepared by sol-gel may be improved when a mixture of methacrylic acid and acetic acid is used. Monophasic, long and almost crack free fibers were prepared at 550 °C when the acid ratio ($\text{CH}_3\text{COOH}/\text{C}_4\text{H}_6\text{O}_2$) is 1/2.

A modification of the methoxyethanol-based sol-gel route was proposed for the deposition of high-quality $\text{PbZr}_{0.53}\text{Ti}_{0.47}\text{O}_3$ (PZT) films at low temperatures. The modification consists of multiple distillations of the Pb precursor after dissolving in 2-methoxyethanol and increasing the pyrolysis temperature after individual layer deposition. In addition, a large PbO excess (20%) was used to maintain the stoichiometry of PZT films. As a result, the films processed at 500 °C exhibited a dielectric permittivity of *ca.* 1900, remanent polarization of *ca.* 30 $\mu\text{C}/\text{cm}^2$ and coercive field of *ca.* 60 kV/cm. The crystallisation mechanism was discussed.

The development of a single perovskite phase in PZT films at low temperature is important, as far as property optimisation and device performance are concerned. A low annealing temperature is also required when metallic (non Pt), glass or polymeric substrates are used. The early stages of nucleation and growth and texture development of the perovskite phase in PZT(52/48) seeded and unseeded sol-gel thin films were studied. TEM and XRD revealed that the perovskite phase nucleates and grows from the film-air interface, surface of the seeds and interface of film-bottom electrode layer in seeded films. In contrast, perovskite nucleation in unseeded films only occurs from the bottom Pt electrode under the same pyrolysis conditions. In addition, the use of seeds encourages a greater nucleation density. The observed local random perovskite nucleation and the decrease of the Pt_xPb phase formation are responsible for the decrease (111) PZT crystalline texture in seeded films. The higher degree of crystallinity and homogeneity of the microstructure of seeded films pyrolysed at low temperatures is patent in the observed dielectric and ferroelectric properties of these films. Seeded PZT thin films pyrolysed at 430 °C for 40 h with a dielectric permittivity of 500 and P_r and E_c of 6.71 $\mu\text{C}/\text{cm}^2$ and 80kV/cm, respectively, are well suited for applications in which glass, metallic or polymeric (such as polyimids) substrates are required.

High quality $\text{SrBi}_2\text{Ta}_2\text{O}_9$ (SBT) single crystals were grown by a self-flux solution method using Bi_2O_3 added with B_2O_3 flux. Chemical composition was $\text{Sr}_x\text{Bi}_y\text{Ta}_2\text{O}_9$, $x=1.03\pm 0.05$, $y=1.87\pm 0.08$. Transparent SBT crystals obtained by slow cooling ($2^\circ\text{C}\cdot\text{h}^{-1}$) of the melt from 1350 °C to 1100 °C exhibit platelet morphology with typical sizes $5\times 3\times 0.05\text{ mm}^3$ dimensions. XRD patterns of SBT single crystals revealed a dominant (001) orientation of a major face and small reflections of non-(001) peaks, arising from twinning defects. Dielectric characterisation showed a phase transition at *ca.* 300 °C with low permittivity values $\epsilon' \approx 120$. Ferroelectric hysteresis measurements along the major face of the crystals showed a saturated hysteresis loop, with a low remanent polarization ($P_r < 0.2\ \mu\text{C}/\text{cm}^2$). Ferroelectricity displayed in the major face of the grown platelets may result from the non-(001) oriented crystallites, *i.e.*, due to the contribution from a-b planes not parallel to the major faces.

A novel chemical procedure was developed to produce SBT powders using Bi and Ta oxides as starting reagents. Briefly, the main steps involved in this method include: (i) preparation of Bi precursor using EDTA, (ii) preparation of a Sr-Ta precursor using citric acid and ethyleneglycol, and (iii) heat treatment of the final mixture of the precursors. A comparative study of this and alternative methods, including the sol-gel method (AC route) and conventional solid-state route was performed: DTA and powder XRD analysis allowed identifying the differences in the pathways involved in those methods. The complete SBT crystallisation was observed at different temperatures for the three methods: highest temperature for SSR method and the lowest one for AC route. Compared to the latter, the novel method produces less aggregated powders. This is an advantage for controlling the morphology of SBT particles to be used as seeds.

Incipient Ferroelectrics. Atomic substitutions in the SrTiO_3 (ST) lattice may change the lattice vibration modes and these changes are expected to depend on the site in which the substitution occurs. In order to discuss the effect of Mg substitution in the ST lattice on the dielectric properties of $\text{Sr}_{1-x}\text{Mg}_x\text{TiO}_3$ and $\text{SrTi}_{1-y}\text{Mg}_y\text{O}_{3-\delta}$ ceramics were studied in the radio frequency (rf), microwave (MW), terahertz (TH) and infrared (IR) range. Micro-Raman spectroscopy and rf tuneability measurements were also conducted. The Micro-Raman spectra and the high frequency dielectric properties of $\text{Sr}_{1-x}\text{Mg}_x\text{TiO}_3$ do not differ considerably from the properties of undoped ST, as well as the field dependence of the permittivity at rf confirming the small, if any, incorporation of Mg into the A-site of ST perovskite. At the same time, B-site Mg doping results in significant hardening of ST lattice, observed in IR reflectivity spectra. Dielectric permittivity and dielectric losses decrease in rf and TH range, corresponding to the decrease of the tuneability and hardening of the ferroelectric soft mode, respectively. In the Raman spectra, the appearance and enhancing of forbidden polar modes TO_4 , at 545 cm^{-1} , and TO_2 , at 174 cm^{-1} , at room temperature, demonstrates the loss of the local inversion centre and breaking of the ST cubic symmetry

by the substitution of Ti^{4+} by Mg^{2+} ions. These results confirm the more favourable occupation by Mg of the Ti site of the ST lattice and show the possibility to utilise the B-site Mg-doped ST as low-loss microwave waveguides or resonators.

Defect Chemistry and Electrical Characteristics of Undoped and Doped ZnO Ceramics. Under normal ceramic processing conditions, ZnO is a n-type semiconductor showing non-linear conduction when doped with Mn and slowly cooled from the sintering temperature. The analysis of the shallow donor was performed at cryogenic temperatures and it was possible to show that this should be the zinc interstitial, with activation energy for conduction of 0.04 eV. Below 18 K hopping conduction dominates.

Magnetostructural Modulation of Strongly Correlated Electric (CMR) Materials

Colossal Magnetoresistive Materials. Work on preparation, structural (X-ray), magnetic, magnetocaloric and electrical properties and radioactive ion local probe studies. Topics: (i) interplay of lattice structure, oxygen vacancy, defects and doping on the magnetic and transport properties of CMR manganites; (ii) physical properties in the vicinity of phase transition; (iii) influence of substrate induced strains on the (magnetic and electric) properties; (iv) studies 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; (v) 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; (vi) study of magnetocaloric effects in manganites in the vicinity of ferromagnetic or charge-order transitions; (vii) theoretical approaches to magnetic materials using generalised thermodynamics; (viii) description of complex systems with long range interactions or distributed characteristic parameters using Tsallis non-extensive statistics; (ix) metallic nanogranular metallic Fe-Cu alloys prepared by ball milling; (x) work on magnetic properties and their relation to composition and structure.

High Tc Superconductors. Work on magnetic and electric properties: critical currents and their relation with structural and phase characteristics in BSCCO fibres.

Advanced Molecular and Supramolecular Materials

C-H...O Hydrogen Bonds: Theoretical and Experimental Studies. The main objective of this project is the study of C-H...O hydrogen bonds and their role in the formation of supramolecular structures, from dimers to large molecular aggregates. The importance of C-H...O hydrogen bonds in the molecular association was assessed for a group of carbonyl containing systems, using *ab initio* calculations and experimental techniques (including vibrational spectroscopy, NMR, Inelastic Neutron Scattering and XRD). Results obtained for simple systems, such as cyclo-pentanone and cyclo-hexanone, present strong evidence of previously ignored C-H...O hydrogen bonds. From these studies, some concepts towards the understanding of the spectroscopic behaviour of C-H...O bonded systems were developed.

Cyclodextrins. β -Cyclodextrin inclusion compounds containing the nonionic surfactants C_mE_n ($C_m=CH_3(CH_2)_{m-1}$; $E_n=(OCH_2CH_2)_nOH$) C_4E_1 , C_4E_2 , C_6E_2 and $C_{12}E_4$ were prepared and characterised by powder XRD, TGA, FTIR and ^{13}C CP MAS NMR, at various relative humidities. These studies point to different types of crystalline structures, depending on the relative sizes of host cavity and guest, and suggest a channel-type structure for the $C_{12}E_4$ inclusion compound.

Equimolar mixtures in deuterated water of β -cyclodextrin (β CD) and decanoic acid, with initial concentration well above its critical micellar concentration, were studied by 1H NMR and the β CD CH protons (H3, H5, H4, H6) used as probes for assessing the effects of varying the concentration of various alkali-metal chlorides (LiCl, NaCl, KCl, CsCl) and sodium salts ($NaClO_4$, NaF, NaCl, NaBr, $NaNO_3$) on the guest inclusion and aggregation/micellisation. NMR studies of the β -cyclodextrin/decanoic acid system in the presence of various cations of group 1 halides were continued and extended to include a trimethylated cyclodextrin. The effect of anions on the β CD-decanoic acid system was also studied.

β -Cyclodextrin (CD) inclusion compounds containing omeprazole nimesulide (NIMED) and ibuprofen were investigated. True inclusion complexes in the solid-state was confirmed by a combination of powder XRD, TGA, FTIR and ^{13}C CP MAS NMR. (i) β -CD inclusion complexes were successfully

prepared with omeprazole and two of the intermediates involved in the synthesis of omeprazole (2-chloromethyl-4-methoxy-3,5-dimethylpyridine-HC and 2-methoxy-2-mercaptobenzimidazole). The experimental results and *ab initio* calculations indicate that the inclusion process involves encapsulation of the benzimidazole fragment in the β -CD cavity. It was found that the interaction with the pyridine fragment is wholly repulsive, due to the presence of several ring substituents. (ii) In the case of NIMED, experimental and theoretical methods have successfully been combined to study the formation of stable inclusion compounds between β -CD and four derivatives of (diphenyl)ether. The inclusion compounds were prepared by co-precipitation from aqueous solution, leading to 2:1 complexes for 2-phenoxybenzene and 2-phenoxyaniline, and 1:1 complexes for the sodium salts of 2-phenoxyethanesulfonamide and nimesulide. In accordance with these results, *ab initio* calculations predict the existence of stable inclusion geometries for these four host-guest systems. The calculations also predict that the formation of stable inclusion geometries for the neutral compounds 2-phenoxyethanesulfonamide and nimesulide is considerably less favourable. This may explain, at least in part, the experimentally observed difficulty in isolating true inclusion compounds containing these guest species. (iii) Suitable crystals for XRD analysis were obtained for an inclusion compound between β -CD and S-ibuprofen. The structure consists of a head-to-head dimer of β -CD molecules stacked along the crystallographic *c*-axis thus forming a slightly tilted channel-type structure. The host-guest interactions were further examined by carrying out *ab initio* calculations.

New Ruthenium Compounds. Conformational studies of Ru(II) complexes incorporating tetrathia-macrocycles were carried out. The synthesis and characterisation of novel polypyridyl ruthenium complexes was continued with a number of new macrocyclic complexes being synthesised via simple substitution reactions and fully characterised by NMR and XRD. Model complexes including DNA bases, such as guanine, were prepared. The interaction of some complexes with DNA and protein transferrin was also been carried out.

Non-Symmetric Macrocycles for Metal Complexes and Supramolecular Aggregates with Pesticides. The main goal of this study is the molecular design and synthesis of macrocycles with novel architectures to be used as sensors for pesticides or to encapsulate heavy atoms, such as Cd, Pb, Hg, UO₂, lanthanides or two small metal ions (Co, Ni or Cu). The synthesis of new sensors for pesticides requires the previous molecular design (molecular mechanics and dynamics calculations) of hosts for specific guests *via* theoretical methods. New macrocycles with large cavities were synthesised and their coordination behaviour with several metal transition ions evaluated and characterised in solution by a range of structural techniques. The structures of some of these complexes were determined by single-crystal XRD.

Molecular modelling studies on cryptand-like ionophores based on a bis calix[4]arene were performed using molecular mechanics and dynamics methods. A range of symmetric and asymmetric calix[4]tubes featuring either alkyl, phenyl or halogen substituents at the upper rim, was studied. The binding properties and selectivity relatively a wide range of metal ions (K⁺, Na⁺, Cs⁺ and Tl⁺) were evaluated. Molecular modelling confirmed that the metal metal cation complexes via the axial route, passing through the calix[4]arene annulus, and provide clear evidence for complexation rate and selectivity of these ligands.

Structural chemistry studies were performed by single-crystal XRD on a wide range of metal complexes having different type of ligands (macrocycles, ally ligands). Some metal complexes were studied by molecular modelling (molecular mechanics and dynamics and/or by DFT calculations).

Organometallic Polynuclear Complexes. Cyanide-bridged polynuclear complexes attract much attention. In 2003 we focused on two issues: (i) characterisation of stable cyanide-isocyanide isomer pairs in M-CN-M' or M-NC-M' bridges, of which only a few examples have been thoroughly characterised; (ii) redox behaviour of LnM-CN-M'L_m complexes, particularly the case where the L and/or L' ligands are redox active species. New isomeric molybdenocene complexes IndCpMo[(μ -CN)Cr(CO)₅]₂ and IndCpMo[(μ -NC)Cr(CO)₅]₂ were prepared and characterized. DFT calculations performed on these trinuclear species as well as on the related cyanide, nitrile and isonitrile complexes and their corresponding anions lead to a rationalisation of several experimental results, namely the redox behaviour. Cyclic voltammetry revealed electronic communication between the metal centres in the heterobimetallic complexes.

Bimetallic Transition Metal Complexes with Bridging Ligands. Heterobimetallic complexes in which metal centres interact through ligand bridges have applications in diverse areas, as variation of metal centres or ligands tailors their spectroscopic and redox properties. [Ru([14]aneS₄)(bpym)](BF₄)₂ was

prepared and characterised by Ru K-edge EXAFS. The crystal structures of the BF_4^- , PF_6^- salts were determined by XRD. Using the cationic core of these compounds as a ‘metalloligand’ starting material, bpym-bridged bimetallic complexes $[\{\text{Ru}([\text{14}]aneS_4)\}_2(\text{bpym})](\text{BF}_4)_4$ and $[\{([\text{14}]aneS_4)\text{Ru}\}(\text{bpym})\{\text{ReO}_3\text{Me}\}](\text{BF}_4)_2$ were prepared and characterised.

Complexes for DNA Probes. Compounds to be used for DNA molecular recognition were synthesised and characterised. Mass spectrometry methods were applied to study their interactions with oligonucleotides. Dinuclear systems with bridging pyridyl ligands were obtained and characterised. The new complex $[\text{Cr}^{\text{III}}[\text{14}]aneN_4(\text{dmsO})\text{Cl}](\text{PF}_6)_2$ was synthesised, its fragmentation mechanism studied by ESMS and XRD structure obtained. This precursor seems to be part of an alternative synthetic route to new heteroleptic $\text{Cr}(\text{N}_6)$ compounds for DNA intercalation.

AREA 2 ADVANCED MATERIALS FOR INDUSTRIAL APPLICATIONS

Reactive Ceramic Components for Process Control

The emphasis of the work was on materials for energy conversion systems, such electrolytes and electrodes for solid oxide fuel cells/SOFCs and other solid state electrochemical applications (e.g. membranes for partial oxidation of hydrocarbons or oxygen separation).

Materials for High-Temperature Electrochemical Applications. The work on SOFC electrolytes was dedicated to materials based on ceria (CGO, CSO), lanthanum gallate, and pyrochlore materials. Micro- or nano-crystalline powders (commercial or prepared) were used to obtain CGO and CSO samples with a wide range of average grain sizes, displaying differences in microstructure-dependent properties. Samples with sub-micrometer grain sizes (down to ca. 100 nm) were prepared with sintering additives added in the form of nitrates (Ni, Co, Cu, Fe). Techniques such as ion blocking, modified emf and faradaic efficiency methods, were used to characterise these materials. Samples with sub-micrometer grain sizes show slightly suppressed n-type conductivity under reducing conditions and an increase in p-type conductivity in air. Impedance spectroscopy was used to characterise the microstructural effects on conductivity, and the differences in grain boundary behaviour between ceria-based electrolytes with different trivalent additives (Gd, Sm, etc.). A combination of coulometric titration and ion blocking was used to study the defect chemistry of CSO and to estimate the mobility and concentration of charge carriers.

Electrolytes with other structure types were also studied (e.g. pyrochlores $Gd_{2-x}Ca_xTi_2O_{7-d}$ and apatites $La_{10-x}(Si,Al)_6O_{26+\delta}$). Their ionic conductivity is poorer than that of ceria- or zirconia-based materials but they are cheaper. Laboratory testing of $Gd_{2-x}Ca_xTi_2O_{7-d}$ electrolytes in SOFC yielded poor power density probably because the ionic conductivity was insufficient and possibly also due to a non-negligible p-type conductivity. Transport properties were measured by emf, faradaic efficiency, oxygen permeability and the dependence of conductivity and Seebeck coefficient vs. oxygen partial pressure and temperature. Transition metal additives or impurities are also responsible for enhanced electronic contributions. Thermal expansion is compatible with other SOFC materials.

There is an increasing interest in ceria containing cermet anodes for SOFC, especially for direct conversion of hydrocarbons. A cellulose precursor method has been developed to process CGO nanocrystalline precursors, fibers, and CGO-metal cermets. Some of these materials were tested as SOFC anodes and as electrocatalysts to promote partial or complete oxidation of methane, without carbon deposition. Cu-CGO cermet anodes were also co-processed and co-fired with a CGO electrolyte, using nanocrystalline powders and sintering additives to densify the electrolyte layer at 1000 °C.

Other ceramic mixed conductors are being studied as potential anodes materials. Though zircon-type $Ce_{1-x}A_xVO_{4-d}$ ($A = Ca, Sr$) seem potential electrocatalysts their transport properties are poor, while their stability under reducing conditions is insufficient. $La_xSr_{1-x}(Ti,Fe)O_{3-d}$ materials were studied for similar reasons and also failed to meet the requirements.

Some alternative cermets included a ceramic phase with proton or proton plus oxygen ion conduction (e.g. $Ni-AZr_{1-x}Y_xO_{3-d}$, $Ni-ACer_{1-x}Y_xO_{3-d}$, $A = Ca, Sr, Ba$). These cermets were prepared by a combustion synthesis method, co-fired with a ceria- or zirconia-based electrolyte layer, and tested with symm

Two alternative materials ($La_2Ni_{0.8}Cu_{0.2}O_{4+d}$ and $Sr_{0.7}Ce_{0.3}MnO_{3-d}$) have been studied as potential novel cathodes for SOFCs. The thermal expansion of these materials agrees better with electrolyte materials than other candidate mixed conducting cathodes, i.e. $(La,Sr)(Co,Fe)O_3$. Higher oxygen permeability was also found for $La_2Ni_{0.8}Cu_{0.2}O_{4+d}$, correlating well with its performance as a cathode, especially after surface modification to enhance surface exchange kinetics. $Sr_{0.7}Ce_{0.3}MnO_{3-d}$ was found to possess electronic conductivity higher than standard $(La,Sr)MnO_3$ and non-negligible increase in ionic conductivity. $Sr_{0.7}Ce_{0.3}MnO_{3-d}$ is an exceptional case of a potential electrode material with n-type conductivity.

Mixed Conducting Materials for Oxygen Separation or Partial Oxidation of Hydrocarbons. This work comprised studies of different mixed conductors based on $LaGaO_3$ with partial substitution of La by Sr and Ga by Mg and/or Fe, Co, Ni. It was found that Sr and Mg acceptors are essential to attain high ionic conductivity but may play a negative role on the surface exchange. Other additives are needed for p-type conductivity. The oxygen transport increases also in the order $Co < Fe < Ni$. Estimated values of a tolerance factor for samples with different additives correlate well with a transition from orthorhombic

to rhombohedral structure and differences in ionic conductivity. The nonstoichiometry of these materials affects their thermal and chemical expansion.

Other studies of mixed conducting materials included composition-structure-microstructure property relations in selected specimens such as $\text{LaCo}_{0.5}\text{M}_{0.5}\text{O}_{3-d}$, $\text{M}=\text{Ni, Fe, Cr}$ $\text{CaTi}_{1-x}\text{Fe}_x\text{O}_{3-d}$, layered materials (e.g. $\text{Sr}_4\text{Fe}_6\text{O}_{13}$), brownmillerite type materials ($\text{CaAl}_{0.5}\text{Fe}_{0.5}\text{O}_{2.5+d}$), and ionic-electronic composites (e.g. $\text{Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{2-d}+\text{La}_{0.8}\text{Sr}_{0.2}\text{Fe}_{0.8}\text{Co}_{0.2}\text{O}_{3-d}$). XRD, Mössbauer spectroscopy and TEM were used for structural characterisation. Oxygen stoichiometry, conductivity and permeability measurements were used to establish correlations between transport properties and structure, including ordering of oxygen vacancies. The emphasis of other work was on stability under reducing conditions, transport properties and surface exchange kinetics of $\text{La}_2\text{Ni}_{0.9}\text{Co}_{0.1}\text{O}_{4+d}$ and $\text{SrCo}_{0.85}\text{Fe}_{0.15}\text{Cr}_{0.05}\text{O}_{3-d}$. The oxygen nonstoichiometry and its effects on stability, defect chemistry and transport properties were also studied.

Oxidation of Methane. This work included studies of complete oxidation in contact with potential solid oxide fuel cell anodes, and partial oxidation of hydrocarbons to obtain synthesis gas (a mixture of CO and H_2), the most important feedstock for commercial Fischer-Tropsch, methanol synthesis, etc. The electrocatalytic activity of mixed conducting materials ($\text{La}_{0.3}\text{Sr}_{0.7}\text{Co}_{0.8}\text{Ga}_{0.2}\text{O}_{3-\delta}$ and $\text{La}_2\text{Ni}_{0.9}\text{Co}_{0.1}\text{O}_{4+\delta}$) has been evaluated for partial oxidation, and nanocrystalline $\text{Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{2-\delta}$ with Pt particles, as a potential anode for direct oxidation of methane in solid oxide fuel cells (SOFC) with yttria-stabilised zirconia electrolyte at 1173 K. Ceria-based anodes lead to high CO_2 selectivity, thus promoting the expected complete oxidation of hydrocarbons in SOFCs. Mixed-conducting membranes also lead to significant formation of CO_2 at 1023-1223 K, requiring the use of suitable catalysts or other modifications to attain better CO selectivity.

The surface exchange limitations of oxygen permeation through dense mixed-conducting membranes enhance membrane stability, enabling the operation of mixed conductors, such as $\text{La}_{0.3}\text{Sr}_{0.7}\text{Co}_{0.8}\text{Ga}_{0.2}\text{O}_{3-\delta}$ (LSCG) and $\text{La}_2\text{Ni}_{0.9}\text{Co}_{0.1}\text{O}_{4+\delta}$ (LNC), under air/dry CH_4 gradient up to temperatures as high as 1173 - 1223 K. Testing of these materials in a model disk-shaped membrane reactor at 1023 - 1223K showed high CO_2 yields (> 75%). In particular, at 1173 K, the CO selectivity was only 17% for LNC and 2% for LSCG ceramics, with methane conversion efficiency of 20 and 37% respectively.

Microstructural Effects. Microstructural effects have been studied for materials with different structure types including those with the structures of perovskite (e.g. $\text{Ca}_{1-x}\text{Ti}_{1-y}\text{Fe}_y\text{O}_{3-d}$ and $(\text{La, Sr})(\text{Ga, Mg})\text{O}_{3-d}$), pyrochlore ($\text{Gd}_{2-x}\text{Ca}_x\text{Ti}_2\text{O}_{7-d}$), and fluorite ($\text{Ce}_{1-x}\text{M}_x\text{O}_{3-d}$, $\text{M}=\text{Gd, Sm}$). The grain boundary effects were characterised by a combination of electron microscopy, impedance spectroscopy and a modified emf technique was also used to distinguish microstructural effects on ionic and electronic contributions. Significant changes in grain boundary behaviour were ascribed to additives and impurities. Certain additives and changes in stoichiometry (e.g. A-site deficiency in $\text{Ca}_{1-x}\text{Ti}_{1-y}\text{Fe}_y\text{O}_{3-d}$) can lower the grain boundary resistance or change their behaviour. Results obtained for ceria- and lanthanum gallate-based materials also indicate that powder preparation and other steps of materials preparation may affect the grain boundary behaviour. Though this is often related to changes in grain size, other important factors were identified (e.g. heterogeneities after powder preparation, segregation, volatilisation, etc.).

Ceramic Composites and Ultra-Hard Coatings for Mechanical Applications

Work concentrated on diamond coatings for tribological applications, colloidal processing of different materials and methods of powder preparation and their characterisation.

Diamond Coatings. Adhesion of diamond castings onto silicon and silicon nitride (Si_3N_4) substrates was evaluated by acoustic emission (AE) assisted Brale indentations. Discrete indentations at different loads were made and the recorded acoustic data correlated with the cracking mechanisms (work assisted by SEM). AE recording distinguished the behaviour of different diamond surface finishing qualities, pointing out to adhesion improvement with the substrate roughness increasing, due to the improvement of the nucleation sites and mechanical interlocking during the deposition process. Previously ground Si_3N_4 substrates (46 mm grit size diamond wheel finishing) could attain nearly 1000 N of load without diamond delamination, this value corresponding to interfacial cracking resistance of 1372 kNm^{-1} . Surface pretreatment procedures were used to improve CVD diamond nucleation. Several mechanical and chemical procedures were accomplished on Si_3N_4 substrates: $1 \mu\text{m}$ or $15 \mu\text{m}$ sized diamond powder scratching or ultrasonical micro-flawing in ethanol or hexane media; cold and hot acid etching; hot basic and CF_4 plasma etching. When chemical pre-treatments were performed, only a few diamond

nuclei were formed because the Si_3N_4 crystals oxidized forming a non-carburising layer of silica that hindered the carbon diffusion into the sample. Unlike the chemical pretreatments, the mechanical preparation was very effective affording high-quality diamond films on Si_3N_4 because the diamond particles tend to incrust in the soft intergranular glassy phase, acting as seeds in promoting diamond nucleation.

X-ray diffraction analysis was used to evaluate residual stresses and CVD diamond texturing. The surface roughness has a net effect on the texture of the films: 15 μm diamond lapped substrates enhanced (220) texture development, contrarily to colloidal silica finished ones. Low incident beam angle X-ray diffraction (LIBAD) and classical $\sin^2\psi$ X-ray diffraction methods also showed that the final stress state depends on the film thickness and substrate surface roughness: average residual stress varied between -0.75 GPa, for 5 μm thick films grown on rough Si_3N_4 substrates, and 0.21 GPa, for 16 μm thick films grown on smooth surfaces. LIBAD analysis allowed discriminating a stress profile along the film thickness, from $\sigma = -3.7$ GPa, at the upper layer of the film, to almost zero, at the film/substrate interface.

Based on the main features given by morphological and mechanical characterisation, a tailored diamond coating of 15 μm thickness on Si_3N_4 round inserts was developed and tested in the dry machining of hardmetal workpieces (WC/25 wt%Co). Preliminary results showed that the depth of cut force is the highest cutting force attaining an initial value of 600 N at $v = 15$ $\text{m}\cdot\text{min}^{-1}$, $f = 0.03$ $\text{mm}\cdot\text{rev}^{-1}$, $d = 0.5$ mm. However, a good workpiece finishing was achieved ($R_a = 0.20$ μm) with very low tool wear, namely by a combination of flank and crater modes with hardmetal deposition on the cutting tool surfaces. Alternatively, sintered WC-Co parts were machined using CVD diamond tipped (by brazing) hardmetal inserts, their behaviour being compared to commercial PCD and c-BN inserts. The CVD diamond tools only presented slight cratering, whereas flank wear was the main wear mode for the other superhard tools. As far as tool wear and workpiece surface are concerned, PCD were the worst of all tested tools, quality. Furthermore, the machining time was reduced to one-tenth with respect to conventional diamond wheel grinding. Having present applications such as face mechanical seals, the ring-on-ring wear tests allowed a better understanding of the sealing and minimum wear conditions of the composites. Silicon nitride-based composites with chemically inert particles were developed for use as cutting tools for iron alloys. Turning tests showed that improvements on the wear resistance are possible using a thermodynamic approach for the stability of silicon based ceramics in contact with steels at high temperature. A correlation was found between the amount of inert particles and the wear resistance evaluated on line using a dynamometer and an in-house developed data acquisition system.

Nanocrystalline diamond (NCD) films were grown using a homemade hot-filament reactor with a new argon line and a two-color pyrometer for filament temperature measurement. The process gas was a mixture of Ar (55-88 %) - H_2 (12-44 %) - CH_4 (0.3-3.9 %), the substrate temperature was kept at 650 $^\circ\text{C}$ or 950 $^\circ\text{C}$, while the filament temperature varied between 2200 $^\circ\text{C}$ and 2450 $^\circ\text{C}$. Continuous, dense, films were obtained on Si_3N_4 substrates using these conditions. The μ -Raman spectra was typical of a NCD structure, characterised by the diamond signature at 1332 cm^{-1} plus a Raman peak at 1150 cm^{-1} and the prolonged shoulder around 1480 cm^{-1} , these two last ones attributed to the trans-polyacetylene structure that is associated to nanodiamond. LIBAD data with a clear peak at $2\theta = 43.9^\circ$, corresponding to the (111) diamond plane, confirmed the presence of diamond.

Colloidal Processing of Materials. Aqueous tape casting was used to obtain crack-free cordierite-glass tapes with a dielectric constant of *ca.* 5 at 1 MHz, with low dielectric loss. This included effects of several experimental factors on all the processing steps.

Stable and high concentrated (≥ 50 vol% solids) aqueous suspensions for colloidal processing were prepared by surface modification of AlN powders. The results achieved are expected to replace colloidal processing in organic-based solvents by processing in aqueous media. High concentration and low viscosity suspensions are the key factors controlling the production of ceramic components through colloidal processing. Green densities higher than 70% of the theoretical density could be obtained by slip casting, and full dense ceramics were obtained by pressureless sintering at 1750 $^\circ\text{C}$. Aqueous processing did not affect the thermal properties of sintered bodies when compared with those processed from organic media.

The influence of several factors on the dispersion ability of reaction sialon precursor powders was studied, in order to establish a reliable methodology for preparing homogeneous, highly concentrated reaction sialon suspension with low viscosity. This included effects of solvent composition, amount of dispersant, mixing procedure, and solids loading on the rheological behaviour of suspensions, slip casting and the microstructure of the green and sintered bodies. The aim was to propose slip casting, tape casting and pressureless sintering to develop high-density reliable α -sialon ceramics with high mechanical properties. Green bodies with high density, homogeneity and improved sinterability could

be obtained, which enabled full dense α -sialon ceramics to be achieved by pressureless-sintering at 1750 °C and reinforced ceramics with elongated α -sialon grains.

The dispersion properties of paper pigments (kaolin, ground calcium carbonate and precipitated calcium carbonate) have been studied in the presence of different dispersants, binders, and carboxymethyl cellulose co-binders. The effects of the same variables on runnability during paper coating and on the final paper properties were evaluated. An adsorption model developed for CMC molecules at the surface of the pigment particles relates the response of colours on coated layers and interactions at microscopic or molecular levels.

Synthesis and Characterisation of Powders. Weakly flocculated aqueous anatase suspensions were *in situ* prepared by hydrothermally treating amorphous titania particles peptized with different amounts of tetraethylammonium hydroxide (TENOH). Formation of hydrous TiO_2 polyanions in the presence of OH^- and tetraethylammonium cations are two essential conditions for the peptization. Transmission electron microscopy (TEM) revealed that the morphology of the particles formed at different TENOH concentrations. Because of the extremely high zeta potential and ionic strength values, non-touching particle networks formed *in situ* in the mother solution in all samples. A trend to coagulation was observed in the suspensions with high concentrations of TENOH, yielding asterisk-like hard agglomerates.

Ti_3AlC_2 powders were prepared by combustion synthesis from low-cost reactants. The combustion behaviour and phase formations in the final products were investigated. The desired product may be obtained through adjusting the initial ratio of the elemental powders. The formation mechanism of ternary phases, Ti_3AlC_2 and Ti_2AlC , consists on the following: preformed TiC crystallites dissolve into the melting Ti-Al composition and then ternary phases precipitate from liquid phase and grow into layers.

Rod-like Y stabilised sialon crystals have been synthesized by combustion synthesis and used as reinforcing agents of reaction α -sialon ceramic matrices. The wear properties of sialon matrix composites were evaluated by a pin-on-disk tribometer under dry conditions. The α -sialon matrix composites were manufactured by slip casting and sintered by uniaxial hot pressing. SEM and energy dispersion spectroscopy were used to analyse the worn surfaces of the α -sialon ceramic composites and the results show that the wear is caused by adhesion and micro abrasion between the rubbing surfaces and is strongly dependent on the amount of reinforcing agent.

Sputtering was also used to coat WC powder particles, as an alternative technique to the conventional mixture of powders. For this work, a stainless steel 304 (ss) coating was sputter deposited on WC powder particles using magnetron sputtering. The results demonstrate that this method is suitable to deposit all the ss elements without uncontrolled changes in stoichiometry. The powder particles were uniformly coated, yielding chemical homogeneity in the distribution of powder constituents. The compaction behaviour showed that it was not necessary to use any type of pressing binder, commonly used in the WC based cemented carbides. The densification of WC-ss powders is higher than that obtained for conventionally prepared composites with identical composition and sintered conditions. Significant weight losses and formation of the ϵ -phase occur at sintering temperatures.

The recycling of industrial wastes (Al-rich sludge, sludges derived from the cutting operations of natural rocks, rubber granulates from tires, etc.) has been studied to produce mullite-based refractories, bricks, gres porcellanato tiles, and sound insulating materials. Lignocellulosic residues of maritime pine, blue gum and cork were used to produce wood-cement composites. The extractive contents of these residues were determined for organic solvents of different polarities. Lignocellulosic materials are richer in polar extractives than in non-polar ones. The behaviour of the lignocellulosic materials in contact with water and with a NaOH 0.1-wt% solution was also studied to simulate the chemical environment of a cement suspension. The effects of lignocellulosic materials in the reaction of cement with water was studied by using calorimetric, X-Rays and thermal techniques to evaluate their effects on cement setting, and on the physical and mechanical properties of the wood-cement composites.

AREA 3

CHEMISTRY AND TECHNOLOGY OF POLYMER AND LIGNOCELLULOSIC MATERIALS AND BIOPOLYMERS

Macromolecular Materials and Lignocellulosics

Lignocellulosics. The studies aiming to understand the chemistry of *Eucalyptus globulus* wood during pulping and bleaching and the comparative study with other hardwoods were pursued. The isolation, purification and characterisation of wood lignins and hemicelluloses and residual lignins and hemicelluloses from unbleached pulps, was concluded. Hemicelluloses from *E. grandis* and *Acacia mangium* were extracted from holocellulose by KOH aqueous solutions or dimethylsulfoxide. The purified xylans were characterised by neutral sugar analysis, methylation analysis, GPC, ¹H NMR and ESI-MS techniques. The analysis of dimethylsulfoxide extracted xylans allowed identifying the position and relative abundance of acetyl groups in these polysaccharides. The peculiar features of the xylans from the different *Eucalyptus* species were clearly evidenced, and explained the higher retention of these hemicelluloses during the kraft pulping process, when compared to the other hardwoods investigated. Wood and pulps lignins were isolated by mild acidolysis and characterised by functional analysis, permanganate oxidation and GPC, ¹H and ¹³C NMR analysis. The ease of delignification of *E. globulus*, when compared to the other wood species, could be assigned to the higher β-O-4 structures, higher S:G ratio and lower degree of condensation of its lignin. Celluloses from woods and unbleached pulps were characterized by X-Ray Diffraction. The evolution of the supramolecular structure of cellulose along the pulping process was investigated. The degree of crystallinity of cellulose as well as the width of crystallites, was shown to increase along the pulping process.

A GC-MS study on the extractives composition of the five hardwoods species and the corresponding ECF beached kraft pulps was conducted. The final bleached pulps showed significantly different extractives contents and compositions, which reflect the composition of the different woods. The surface composition of such fibres was assessed by ESCA and ToF-SIMS (in cooperation with Abo Akademi, Turku, Finland) and compared with the bulk composition of fibres. Significant differences were observed between fibres and between surface and bulk composition, particularly in the case of extractives.

Studies aiming to improve polysaccharides retention and thus improving the yield of pulp during *E. globulus* kraft pulping were initiated. The screening of potential modifications of the kraft process, aiming to improve pulp yield was investigated. These included (i) early interruption of the kraft pulping, followed by oxygen delignification stage(s), (ii) impregnation stages with white liquor, including or not surfactants and/or anthraquinone (iii) levelling of the alkaline charge along the pulping process. Results obtained so far, show that pulps yield may be improved 1-2% by using different combinations of those modifications. In parallel, a study aiming to understand the behaviour of black liquor dissolved xylans in the last stages of the cooking (looking for possibilities for their re-precipitation at the fibres surfaces) was initiated. Black liquors from different stages of the kraft process were produced and analysed. Xylans were selectively recovered. The characterisation of the xylan thus obtained was initiated, involving sugar analysis, methylation (linkage) analysis, ¹H NMR, ESI-MS and GPC. The results obtained so far show that dissolved xylans have average molecular weights in the range 13-15 KDa, and structures bearing different types and abundances of uronic acid substituents, thus opening new perspectives for their re-precipitation at the fibres surface, increasing pulp yield.

The structural changes of xylan in sulphite *Eucalyptus globulus* pulp during pulping and P(O)P bleaching have been investigated. The influence of the washing efficiency on the bleaching of sulphite pulp in P(O)P sequence has been investigated. The simulation of different washing efficiency of unbleached pulp allowed to conclude that the pulp brightness in P(O)P sequence is not affected drastically when the former varied around 80-95% (around 89% ISO). The increase of washing efficiency to 99% (implementation of a second step of washing equipment) did not lead to substantial brightness increase.

New pathways for the synthesis of 5-5' dilignols have been developed. This allowed the study of fragmentation patterns of such kind of substructures in ESI-MS/MS experiments and their reliable identification in lignin.

Research on the nature of lignin-carbohydrate complexes in eucalypt wood was started. The LCC structures in *E. globulus* were assessed using the technique of ¹³C selective labeling in combination with advanced NMR techniques. ¹³C-[β] or ¹³C-[α] labeled lignin precursors (coniferin and syringin) were

administered in cut shoots from their aqueous solutions. $^{13}\text{C}[\alpha]/^{13}\text{C}[\beta]$ enriched/non-enriched LCC were studied without their isolation by solid state ^{13}C NMR or were isolated from newly soft xylem and studied by liquid state NMR. The LCC structures were elucidated editing the difference ^{13}C NMR spectra of labeled/non-labeled samples and applying different 2D/3D NMR techniques.

Aiming at promoting a research work on the reliable detection of muconic acid structures in biodegraded or chemically oxidised lignins, a series of lignin model compounds of muconic acid type were synthesised and characterised by FTIR, NMR, ESI-MS.

A series of polyoxometalates (POMs), namely mono-substituted of Keggin-type anions (α - $[\text{SiW}_{(12-n)}\text{Mn}^{\text{III}}(\text{H}_2\text{O})_n\text{O}_{(40-n)}]^{(4+n)-}$ ($n = 1, 2$) and α - $[\text{XW}_{11}\text{M}(\text{H}_2\text{O})\text{O}_{39}]^{n-}$ ($\text{X} = \text{Si}, \text{B}, \text{M} = \text{Co}^{\text{III}}$; $\text{X} = \text{Si}, \text{P}, \text{M} = \text{Ru}^{\text{IV}}$) and a sandwich-type (α - $\text{B}-(\text{PW}_9\text{O}_{34})_2\text{Mn}^{\text{II}}_{(4-n)}\text{Mn}^{\text{III}}_n(\text{H}_2\text{O})_2]^{(10-n)-}$ ($n = 1$ or 3)) have been synthesised and characterised. POMs were tested as catalysts in oxygen delignification. All POMs showed catalytic activity. However, the poor re-oxidation of reduced POMs with oxygen did not allow a high delignification degree. A combinatory approach was proposed using POMs and laccase of *Trametes versicolor* in a multi-stage system for the oxygen bleaching. Highly effective and selective delignification was achieved with α - $[\text{SiW}_{11}\text{Mn}^{\text{III}}(\text{H}_2\text{O})\text{O}_{39}]^{5-}$, α - $[\text{SiW}_{10}\text{Mn}^{\text{III}}_2(\text{H}_2\text{O})_2\text{O}_{38}]^{6-}$ and α - $[\text{SiW}_{11}\text{Co}^{\text{III}}(\text{H}_2\text{O})\text{O}_{39}]^{5-}$.

The application of the Py-GC-MS (pyrolysis coupled with GC-MS) technique to the fast characterisation of wood and pulp components as well as samples from the industrial papermaking processes was initiated. The technique was optimised for the rapid determination of syringyl:guaiacyl ratios of wood and pulps lignins. The characterisation of paper additives and industrial pitch samples was initiated.

A new research programme aiming to improve the performance of cellulosic fibres on paper and new fibre-based composite materials was initiated. This involves (i) the surface modification of fibres in order to induce surface thermoplasticity, to render the surface reactive or compatible with apolar polymeric matrices, (ii) the deposition of nano-particles (ZnO , TiO_2 , BiVO_4 , among others) at the fibre structure and (iii) the development of new silica-cellulose fibre based materials. The study on the surface cellulose esterification with fatty acids has been initiated using a cellulose/fatty acyl chlorides/pyridine reaction system. The effect of the solvent, reaction time and fatty acids chain length on the extent of esterification and on the properties of the obtained cellulose derivatives was evaluated. The characterisation of the modified fibres was initiated by IR and contact angle measurement. Some preliminary composites samples with modified fibres and polypropylene were prepared. The deposition of BiVO_4 nano-particles in the cellulose fibres structure was successfully demonstrated. The characterisation of the structure/composition of raw materials (primary sludge, bleached/non-bleached and beaten/non-beaten eucalypt kraft pulps) for the silica-cellulose fibre materials has been accomplished. The optimisation of the sol-gel synthesis to produce new silica-cellulose hybrids was done. The materials obtained were characterised by a series of thermal analysis (TDA, DSC) and spectroscopic techniques (FTIR, NMR (^{13}C , ^{29}Si), Raman). The image analysis was carried out using optic microscope, SEM, AFM. The first steps on the development of techniques for the preparation of silica-cellulose hybrid materials with specific physical and acoustic properties were accomplished. Multidimensional NMR studies for structure determination of lignocellulosic materials have been continued.

Other Polymer Systems and Materials. Studies were initiated focusing on the preparation of polymer/ SiO_2 and polymer/silica coated nanocomposites *via in situ* polymerisation using emulsion and or miniemulsion polymerisation techniques. The effect of a series of parameters was investigated and optimised both for emulsion and miniemulsion. PS based nanocomposites containing SiO_2 , $\text{Bi}_2\text{S}_3@ \text{SiO}_2$ and Q-dots@TOPO have been prepared and characterised. A literature survey on the RAFT mechanism with emphasis on miniemulsion has also been done which will allow the development of more efficient routes for the preparation of nanocomposites. PPy/ SiO_2 nanocomposites were prepared by emulsion polymerisation and characterised. The effect of the fillers on the thermal and electric properties proved very interesting.

Regarding work on exo-polysaccharides produced by micro-organisms under a variety of fermentation conditions, the purification procedure was optimised and most of the materials characterised.

In the synthesis of liquid polyols and polyurethanes from solid cork residues, the study of the oxypropylation reaction has been concluded, and polyurethane foams have been prepared with good structural and mechanical properties.

Polymer materials, quantitative experimental creep and theoretical non-simulative molecular dynamics studies were continued, with the development and initial validation of a cooperative segmental theory of molecular dynamics and a closely related non-linear creep model.

Attention has been devoted to paraffin crystallisation. Studies of crystal structure, crystal growth and rheology have been carried out aiming at the use of these materials in energy storage and insulation. Some effort has also been addressed towards the measurement and modelling of vapour-liquid equilibrium of polymer solutions, but the main focus remained on the behaviour of biodegradable and natural polymers capable of replacing standard polymers in food packaging.

Biomaterials

Biological, Structural and Identification FTIR, NMR and Other Studies. New adducts of Cr(V) were tested in *in vivo* with mice submitted to severe or chronic intoxication, to characterise degenerative damages in organs by histological, histochemical and ultrastructural methods. Cytometry and fluorescence microscopy techniques were also used.

The chitosan-cardosin association, as relevant factors for the prevention of fibrosis after peritoneal surgery, was tested *in vivo* studies. Biochemical, histological and ultrastructural methods were used to evaluate the response of some target organs with different functions (metabolic, excretion, and immune). Studies were also conducted in order to immobilize cardosins within membranes, sponges and microspheres based on chitosan for a controlled release of the enzyme within the peritoneal region. The effect of some ions released from biomaterials such as titanium and Cr-Co-Mo based alloys were investigated in mice using cryogenic sections of relevant organs such as the spleen, the kidney, and the liver. Histochemistry for proteins and carbohydrates were also used.

State-of-the-art NMR techniques were applied to liquid complex mixtures (foodstuffs, biofluids), and solid carbohydrates. The fast and unambiguous characterisation of tens of metabolites in liquid mixtures was achieved by LC-NMR/MS and by diffusion-ordered spectroscopy; this has important applications in the food industry and some present work is based on contacts with Heineken and Unicer for on-line applications. In the solid state, homo- and heteronuclear correlation experiments based on new decoupling schemes have been applied to the characterisation of solid glucose, maltose and trehalose in either crystalline, amorphous or glassy states. Changes upon heating/cooling were followed by NMR and other methods (DSC, Raman, FTIR). Finally, some work has focused on the use of NMR to identify the nature and dynamics of mannan gel networks.

The NMR study of biomolecules containing paramagnetic metal centres was continued. Pseudocontact shifts were measured for Ni substituted, $^{13}\text{C}/^{15}\text{N}$ labelled rubredoxin (Rd). The structure in solution has been determined.

The perdeuteration (replacement of ^1H by D) of 5-Aminolevulinate Synthase (POCTI/BME/39184/2001) has been carried out and improvements in spectral resolution have been seen in TROSY type experiments. TROSY experiments have also been used to initiate the backbone assignment of labelled Heme Binding Protein (Brian Volkman, Univ. Wisc. Milwaukee, EUA)

NMR relaxation studies of novel biomedical membranes have been initiated in order to probe the type of interactions occurring between the polysaccharide and protein that make up the polymer matrix and to relate these to the physical properties of the membranes.

Diffusion ordered spectroscopy (DOSY) has been developed and applied to complex mixtures (beer, port wine, ligand/protein) allowing the spectral separation of components by diffusion coefficient.

Glass and Ceramic-Based Biomaterials. The role of albumin in the mineralisation process of commercial hydroxyapatite and synthesised biphasic (hydroxyapatite-tricalcium phosphate) ceramics in a bufferless simulated inorganic plasma (HBSS) was investigated by conventional *in vitro* tests and static and dynamic wettability measurements. Albumin was either pre-adsorbed or solubilised in HBSS. It was found that calcium complexation by albumin plays a key role in early mineralisation kinetics, so that mineralisation is favoured when albumin is pre-adsorbed and hindered when it is dissolved in HBSS. In the biphasic ceramic this picture is complicated by the fact that albumin, in solution, seems to promote the dissolution of tricalcium phosphate, and simultaneously compete for calcium with the ceramic. It also appears that albumin has a stabilising effect of octacalcium phosphate present in deposits on commercial hydroxyapatite. The same effect may be present in the case of the biphasic ceramic, at earlier mineralisation times, when octacalcium phosphate appears as a precursor of hydroxyapatite. Octacalcium phosphate formation on commercial apatite is accompanied by carbonate substitution in phosphate positions.

The substitution of Tris/HCl buffer by $\text{CO}_2/\text{HCO}_3^-$ buffer in SBF was studied. An appropriate gas mixture of CO_2/N_2 was continuously bubbled in SBF solution prepared without addition of Tris/HCl. This method renders possible to buffer the solution in the 7.3 – 7.4 pH interval and at the same time reach a HCO_3^- concentration between 24 and 27 $\text{mmol}\cdot\text{dm}^{-3}$, which are the normal concentration values in the blood plasma. Mineralisation studies of calcium phosphates ceramics using this solution showed

that, in the presence of this HCO_3^- concentration, the formation of a mineralisation layer in the ceramic surface is done via a carbonated OCP phase, which then evolves to carbonated hydroxyapatite. With normal Tris/HCl buffered SBF OCP phase was not detected. These few results strongly suggest that mineralisation studies in this modified SBF mimetic biomineralization more closely than traditional SBF.

Two ceramic phosphates, commercial hydroxyapatite and synthesised biphasic hydroxyapatite-14 wt.% alfa-tricalcium phosphate were incubated in Hank's balanced salt solution (HBSS) and Kokubo's simulated body fluid (SBF) at 37 °C and the respective surface modifications investigated. The static contact angles (SCA) of water and diiodomethane on the surfaces of both incubated and non-incubated materials were measured as a function of time, showing that surface modifications were different for each type of phosphate and depended on the incubating solution. Dynamic contact angle (DCA) hysteresis provided information on the characteristics of possible deposits. These studies were complemented with SEM/EDS, FT-IR and XRD analysis of the surfaces. Compositional changes in the incubating solutions with time were monitored by ICP spectroscopy. The main conclusion is that the formation of calcium phosphate deposits in non-buffered solutions, like HBSS, is clearly influenced by an uncontrolled pH increase with time. Another conclusion is that wettability measurements, especially DCA, provide a most sensitive method to detect surface transformations leading to mineralisation.

The influence of solution composition (pH, presence of Na, K, Mg and Cl ions) and temperature on the crystallization and ageing of the calcium phosphate solid phases was investigated and the aqueous solutions were studied by ICP. The composition of the solid phases was determined by wet analysis and by X ray diffraction, thermogravimetry and infrared spectroscopy. As was expected these parameters have a small influence on the crystallized phases and the ageing of the different solids under physiologic simulated conditions shows the appearance of deficient hydroxyapatite solid solutions with the ions of the solution.

Optimisation of the processing conditions of hydroxyapatite–alumina composites by DCC, for a constant addition of substrate, allow to evaluate the amount of enzyme that leads to the obtention of wet coagulated green bodies with higher compressive strengths and a with a short coagulation time.

Porous apatite particles produced by spray drying a suspension of apatite nanoparticles were incorporated in the macroporous scaffold structure of PLGA and PLGA-CaP composite, previously apatite coated by the biomimetic method. It has been shown the capability of the so produced spray dried apatite particles to adsorb and release a model drug compound in solutions at physiological pH and temperature.

Composites of brushite-chitosan have been obtained by freeze-drying of chitosan solutions and calcium and phosphorous solutions.

Process Development and Optimisation

Phase Behaviour and Transport Properties Relevant in Environmental Protection, Chemical Processing and New Materials Production. A new project entitled Simulation of Cyclic Separation using Parallel Computing started on 10/11/03. One CPU was configured as a server, where the main services of the cluster system will be located. Basically, common net services as DHCP, NIS, NFS, BIND, NTP were installed and configured. Also, a slave node was configured for accessing the master node. All this work is mainly “software administration” but it is important because these services coordinate the groups of machines. After the server and node become stable, the remaining computers will be installed by replication. Libraries and the main languages of choice were selected. The old SAXS for cyclic separation process simulator was revisited and recompiled.

Further work has been carried out on binary diffusion coefficients in supercritical carbon dioxide, and dynamic and equilibrium adsorption experiments.

On the hydrodynamic behaviour of liquid-liquid dispersions, new experimental data and modelling results of drop size distributions in agitated contactors were obtained.

Synthesis of New Materials. The activities with biologic reactors follow two approaches: the production of macromolecules (biopolymers and enzymes); and the use of unconventional solvents to enhance the aeration of the reactor aiming at an increase of the production rates. During 2003, the conditions for the production of a biopolymer from *Trametes versicolor* were optimised and the polymer characterised. Also, using *Trametes versicolor*, the production of laccase was optimised on a batch CSTR. Laccase was used for effluent treatment of textile industries with good results.

The oxidation of cis-pinane to 2-pinane hydroperoxide and the subsequent reduction to 2-pinanol are two steps of the so-called “ α -pinene route” for the synthesis of more valuable aromas such as linalool, nerol and geraniol. The oxidation of cis-pinane with *tert*-butyl hydroperoxide, at room temperature and

atmospheric pressure in the presence of iron-phthalocyanines supported on activated carbons produces mainly 2-pinane hydroperoxide (77% selectivity at 91% conversion). The influence of the surface chemistry of the carbon supports on catalytic activity and product selectivity was studied. The catalysts prepared from supports with very high or very low oxygen content exhibit low activity, whereas for supports with intermediate oxygen contents a good correlation between the amount of phenols and lactones and catalytic activity was obtained.

PRODUÇÃO

CIENTÍFICA

2003

PRODUÇÃO CIENTÍFICA 2003

Teses de Doutoramento	13
Teses de Mestrado	8
Artigos SCI IF>5	3
Artigos SCI IF<5	221
Artigos não SCI	26
Capítulos de Livros (Ed. Internacional)	5
Capítulos de Livros (Ed. Nacional)	9
Patentes Nacionais	3
Proceedings de Conferência Internacional (nº pág. ≥4)	51
Proceedings de Conferência Nacional ou Internacional (nº pág.<4)	196
Outras Publicações	10
Organização de Congressos Internacionais	4
Organização de Congressos Nacionais	1
Organização de Cursos, Seminários e Programas de Formação	2
Actividades de Extensão	17
Projectos	100

PRODUÇÃO CIENTÍFICA

31 de Dezembro de 2003

TESES DE DOUTORAMENTO

A CICLODEXTRINA-BETA NA FORMAÇÃO DE COMPLEXOS DE INCLUSÃO
E DE NOVAS ESTRUTURAS SUPRAMOLECULARES

BRAGA S S

SUPERVISOR: TEIXEIRA DIAS, J J C

UNIVERSIDADE DE AVEIRO 2003.

ESTUDO DA FORMAÇÃO DE DEPÓSITOS PARAFÍNICOS EM FLUIDOS
PETROLÍFEROS A ALTAS PRESSÕES

SANSOT J M- ‘. DOUTORAMENTO EM FÍSICA,

SUPERVISORES: COUTINHO JAP, DARIDON JL

UNIVERSIDADE DE AVEIRO – UNIVERSITÉ DE PAU ET DES PAYS DE
L’ADOUR, FRANÇA, 2003.

ESTUDO DE LIGAÇÕES DE HIDROGÉNIO C-H...O EM LÍQUIDOS

VAZ P M D

SUPERVISOR: RIBEIRO-CLARO P J A

UNIVERSIDADE DE AVEIRO 2003.

ESTUDOS ESTRUTURAIS POR RMN DE PROTEÍNAS CONTENDO CENTROS
FERRO-ENXOFRE [Fe- 4S]

NUNES SHGC

SUPERVISORES: GOODFELLOW BJ; MOURA I

UNIVERSIDADE NOVA DE LISBOA 2003.

EUCALYPTUS GLOBULUS LOW MOLECULAR WEIGHT ORGANIC
COMPOUNDS: BEHAVIOUR DURING WOOD KRAFT PULPING AND PULP
BLEACHING.

FREIRE BARROS C S R

SUPERVISORES: NETO C P; SILVESTRE A J D

UNIVERSIDADE DE AVEIRO 2003.

HIGH-RESOLUTION AND HETERONUCLEAR CORRELATION NMR
TECHNIQUES FOR THE STUDY OF QUADRUPOLAR NUCLEI IN SOLIDS
MORAIS C M

SUPERVISORES: ROCHA J; FERNANDEZ C
UNIVERSIDADES DE AVEIRO E CAEN 2003.

INFLUÊNCIA DA COMPOSIÇÃO E ESTRUTURA DOS COMPONENTES
DA PASTA KRAFT NA SUA BRANQUEABILIDADE

DANIEL A I
SUPERVISORES: NETO C P AND EVTUGUIN DV
UNIVERSIDADE DE AVEIRO 2003.

INFLUENCIA DA COMPOSIÇÃO E ESTRUTURA DOS COMPONENTES DA
PASTA KRAFT NA SUA BRANQUEABILIDADE.

DANIEL A I D
SUPERVISORES: NETO C P; EVTUGUIN D V; SILVESTRE A J D
UNIVERSIDADE DE AVEIRO 2003.

INFLUÊNCIA DOS CLORETOS DE SÓDIO, POTÁSSIO E MAGNÉSIO NA
FORMAÇÃO DA HIDROXIAPATITE E SEUS PRECURSORES

INÁCIO P G D
SUPERVISOR: MAGALHÃES M C F
UNIVERSIDADE DE AVEIRO 2003

OPTIMIZAÇÃO DAS CONDIÇÕES DE PROCESSAMENTO DE MATERIAIS
FILTRANTES À BASE DE ARGILA PARA PURIFICAÇÃO DE ÁGUA E
REMOÇÃO DE METAIS PESADOS

VENTURA J M
SUPERVISOR: LABRINCHA J A
UNIVERSIDADE DE AVEIRO 2003.

OXO-ORGANOCOMPLEXOS SUPTADOS EM MATERIAS MESOPOROSOS.
PREPARAÇÃO, CARACTERIZAÇÃO E ACTIVIDADE CATALÍTICA

NUNES C M D
SUPERVISORES: GONÇALVES IS
UNIVERSIDADE DE AVEIRO 2003.

REACÇÕES DE SUPERFÍCIE DE CERÂMICOS DE FOSFATO DE CÁLCIO EM
PLAMA SIMULADO

MARQUES P A A P
SUPERVISORES: CORREIA R N, MAGALHÃES M C F
UNIVERSIDADE DE AVEIRO 2003.

SÍNTESE E CARACTERIZAÇÃO DE NANOESTRUTURAS DE
SEMICONDUCTORES

MONTEIRO O C
SUPERVISOR: TRINDADE T
UNIVERSIDADE DE AVEIRO 2003

TESES DE MESTRADO

AVALIAÇÃO *IN VIVO* DO EFEITO PROTECTOR DE ANTIOXIDANTES NA EXPRESSÃO DA TOXICIDADE DE ARSENICAIS INORGÂNICOS
SUPERVISORES: PEREIRA M L; BASTOS M L
UNIVERSIDADE DE AVEIRO 2003.

ESTRUTURA E MAGNETISMO DE NANOHÍBRIDOS DI-UREASILS DOPADOS COM FERRO E NEODÍMIO
SILVA, NUNO JOÃO OLIVEIRA E
SUPERVISORES: AMARAL V S; CARLOS L D
UNIVERSIDADE DE AVEIRO FEV 2003.

NOVOS PIGMENTOS À BASE DE BISMUTO
NEVES M C
SUPERVISOR: TRINDADE T
UNIVERSIDADE DE AVEIRO 2003

NOVOS SISTEMAS LUMINESCENTES DE POLIOXOMETALATOS CONTENDO LANTANÍDEOS
SOUSA; F L
SUPERVISORES: CAVALEIRO; A M V; NOGUEIRA, H S;
UNIVERSIDADE DE AVEIRO 2003.

O TIMO: ÓRGÃO ALVO DA TOXICIDADE DE METAIS
SUPERVISORES: PEREIRA M L; FERREIRA M E
UNIVERSIDADE DE AVEIRO 2003.

PREPARAÇÃO DE SIALON'S REFORÇADOS COM PARTÍCULAS ALONGADAS DE SIALON OBTIDAS POR SÍNTESE POR COMBUSTÃO (CS)
FILHO X V L
SUPERVISORES: FERREIRA J M F;
UNIVERSIDADE DE AVEIRO 2003.

RECICLAGEM DE CINZAS VOLANTES POR VITROCERAMIZAÇÃO
MARTA ASCENSÃO CARMONA FERRO,
MESTRE EM CIÊNCIA E ENGENHARIA DE MATERIAIS,
UNIVERSIDADE DE AVEIRO, 2003.

SÍNTESE DE PIGMENTOS ESTRUTURADOS QUIMICAMENTE: CAULINO E CARBONATO DE CÁLCIO
CONCEIÇÃO S
SUPERVISORES: FERREIRA J M F; VELHO J L
UNIVERSIDADE DE AVEIRO 2003.

ARTIGOS SCI, IF \geq 5

BIS(CALIX[4]DIQUINONE) RECEPTORS: CESIUM- AND RUBIDIUM-
SELECTIVE REDOX-ACTIVE IONOPHORES

WEBBER P. R. A.; BEER P. D.; CHEN G. Z.; FELIX V.; DREW M. G. B.
J. AMER. CHEM. SOC
2003, 125(19), PP 5774-5785

MULTIFUNCTIONAL SODIUM LANTHANIDE SILICATES: FROM BLUE
EMITTERS AND INFRARED S-BAND AMPLIFIERS TO X-RAY PHOSPHORS

ANANIAS D; FERREIRA A; CARLOS L D AND ROCHA J
ADV MATER
2003, 15, PP 980-85.

NOVEL MICROPOROUS LANTHANIDE SILICATES WITH TOBERMORITE-
LIKE STRUCTURE

FERREIRA A; ANANIAS D; CARLOS L D; MORAIS C M AND ROCHA J
J AM CHEM SOC
2003, 125, PP 14573-14579.

ARTIGOS SCI, IF $<$ 5

A NEW CORRESPONDING STATES MODEL FOR THE ESTIMATION OF
THERMOPHYSICAL PROPERTIES OF LONG CHAIN N-ALKANES

QUEIMADA A.J., STENBY E.H., MARRUCHO I.M., COUTINHO, J.A.P.
FLUID PHASE EQUILIBRIA
2003, 212, PP 303-314.

AB INITIO STRUCTURE DETERMINATION OF NOVEL SMALL-PORE
METAL-SILICATES: KNOTS-AND-CROSSES STRUCTURES

LIN Z; FERREIRA A; SOARES M R AND ROCHA J
INORG CHIM ACTA
2003, 356, PP 19-26.

ACOUSTIC EMISSION DETECTION OF MACRO-INDENTATION CRACKING
OF DIAMOND COATED SILICON

BELMONTE M ; FERNANDES AJS; COSTA FM; OLIVEIRA FJ AND SILVA RF
DIAM RELAT MATER
2003, 12, 10-11, PP 1744-1749.

AEROSOL ASSISTED-METALLO-ORGANIC CHEMICAL VAPOR DEPOSITION
(AA-MOCVD) OF Bi_2Se_3 FILMS USING SINGLE-MOLECULE PRECURSORS.
THE X-RAY CRYSTAL STRUCTURE OF BISMUTH (III)

DIBUTYLDISELENOCARBAMATE,
MONTEIRO O. C.; TRINDADE T.; ALMEIDA PAZ F. A.; KLINOWSKI J.;
WATERS J.; O'BRIEN P.
J. MATER. CHEM.
2003, 13, PP 3006-3010.

ADHESION BEHAVIOUR ASSESSMENT ON DIAMOND COATED SILICON
NITRIDE BY ACOUSTIC EMISSION

BELMONTE M ; FERNANDES AJS; COSTA FM; OLIVEIRA FJ AND SILVA RF
DIAM RELAT MATER
2003, 12, 3-7, PP 733-737

AG(I) AND CU(I) COMPLEXES OF ETAMETHYLDIPHOSPHINEDISULFIDE:
SYNTHESIS AND STRUCTURE

LIU H. CALHORDA M. J.; DREW M.G.B.; FELIX V.
INORGANICA CHIMICA ACTA
2003, 347, PP 175-180

α -SIALON CERAMICS OBTAINED BY SLIP CASTING AND PRESSURELESS
SINTERING

XIN X; OLIVEIRA M I L L, AND FERREIRA J M F
J AM CERAM SOC
2003, 86, PP 366-368.

ANALYSIS OF THE COMPOSITION INDUCED TRANSITION FROM RELAXOR
TO FERROELECTRIC STATE IN $\text{Pb}(\text{Fe}_{2/3}\text{W}_{1/3})\text{O}_3 - \text{PbTiO}_3$ SOLID
SOLUTIONS

L. MITOSERIU, A. STANCU, C. FEDOR, P. M. VILARINHO
JOURNAL OF APPLIED PHYSICS
2003, 94, 3, PP 1918 – 1925.

ANION-DEFICIENT PEROVSKITE $\text{Pb}(\text{Mg}_{0.5}\text{Nb}_{0.5})\text{O}_{2.75}$ CERAMICS OBTAINED
UNDER HIGH PRESSURE,

SALAK A N, VYSHATKO N P, FERREIRA V M, RADYUSH Y V,
OLEKHNOVICH NM,
FERROELECTRICS,
2003, 296, PP 175-186.

APPLICATION OF ELECTROSPRAY IONIZATION MASS SPECTROMETRY TO
THE ELUCIDATION OF THE PRIMARY STRUCTURE OF LIGNIN.

EVTUGUIN D V; AMADO F M L
MACROMOL. BIOSCI.
2003, 3 (6) PP 339-343

APPLICATION OF NMR SPECTROSCOPY AND LC-NMR/MS TO THE
IDENTIFICATION OF CARBOHYDRATES IN BEER

DUARTE, I.F.; GODEJOHANN, M.; BRAUMANN, U. ; SPRAUL, M; GIL, A.M.

JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY,
2003, 51, 4847-4852.

AQUEOUS PROCESSING OF CERAMIC AND GLASS-CERAMIC
SUBSTRATES: THE FUTURE TRENDS IN TAPE CASTING TECHNOLOGY
FERREIRA J M F; MEI S AND GUEDES M
MATERIALS SCIENCE FORUM
2003, 442-442, PP 27-36.

ASSESSING THE POTENTIAL OF FAST AMPLITUDE MODULATION PULSES
FOR IMPROVING TRIPLE-QUANTUM MAS NMR SPECTRA OF HALF-
INTEGER QUADRUPOLAR NUCLEI
MORAIS C M; LOPES M; FERNANDEZ C AND ROCHA, J.
MAGN RESON CHEM
2003, 41, PP 679-688.

BARIUM METAPLUMBATE THIN FILM ELECTRODES FOR
FERROELECTRIC DEVICES
MARDARE A. I., MARDARE C. C., JOANNI E., FERNANDES J. R. A.,
VILARINHO P. M., KHOLKIN A. L.
FERROELECTRICS
2003, 293, PP 177-188

BIMETALLIC TRANSITION METAL-RUTHENIUM(II) COMPLEXES WITH
BRIDGING BIPYRIMIDINE LIGANDS
NUNES C D; PILLINGER M; HAZELL A; JEPSEN J; SANTOS T M;
MADUREIRA J; LOPES A D; GONÇALVES I S
POLYHEDRON
2003, 22 PP 2799-2807.

BULK AND GRAIN BOUNDARY CONDUCTIVITY OF $\text{Ca}_{0.97}\text{Ti}_{1-x}\text{Fe}_x\text{O}_{3-D}$
MATERIALS
CHINARRO E, FIGUEIREDO F M, JURADO J R, FRADE J R
SOLID STATE IONICS
2003. 160, PP 161-168

C-H...O HYDROGEN BONDS IN LIQUID CYCLOHEXANONE REVEALED BY
THE NC=O SPLITTING AND THE NC-H BLUE SHIFT
VAZ P D; RIBEIRO-CLARO P J A
J. RAMAN SPECTROSC. 2003, 34, PP 863-867

CARBOHYDRATE-DERIVED CHLORINATED COMPOUNDS IN ECF
BLEACHING OF HARDWOOD PULPS: FORMATION, DEGRADATION AND
CONTRIBUTION TO AOX IN A BLEACHED KRAFT PULP MILL
FREIRE C S R.; SILVESTRE A J D AND NETO C P
ENVIRON SCI TECHNOL
2003, 37, PP 811-814.

CATENA-(1,3-DIAMMONIOPROPANE PHOSPHATO)-TRIOXO-TRIVANADIUM REDETERMINATION AT 180(2) K
PAZ F A A; SHI F; TRINDADE T; ROCHA J AND KLINOWSKI J
ACTA CHRYSTAL E
2003, E59, PP M179-M182.

BIS(μ_2 -HIDROXO)-BIS(μ_4 -DIHYDRATE): A

CATION COORDINATION IN MONO-URETHANESIL HYBRIDS DOPED WITH SODIUM TRIFLATE
GONÇALVES M C, BERMUDEZ DE ZEA V, OSTROVSKII D, CARLOS L D
ELECTROCHIMICA ACTA
2003, 48(14-16), PP 1977-1989.

CERAMIC IN VITRO MINERALISATION PROTOCOLS: A SUPERSATURATION PROBLEM
MARQUES PA A P; MAGALHÃES M C F; CORREIA R N; MARTIN A I; SALINAS A J; VALLET-REGÍ M
KEY ENG MATER
2003, 254-256, PP 143-146

CHARACTERIZATION OF ACETYLATED HETEROXYLAN FROM *EUCALYPTUS GLOBULUS* LABILL
EVTUGUIN D V; TOMÁS J L; SILVA A M S; PASCOAL NETO C
CARBOHYDR. RES.
2003, 338 (7) PP 597-607

CHARACTERISATION OF THE AROMATIC COMPOSITION OF SOME LIQUID FOODS BY NMR SPECTROSCOPY AND LC-NMR/MS
GIL, A.M.; DUARTE, I.F. ; GODEJOHANN, M.; BRAUMANN, U.; SPRAUL, M.
ANALYTICA CHIMICA ACTA,
2003, 488/1, 35-51.

CHEMICAL BATH DEPOSITION OF CERIUM DOPED BIVO₄
NEVES.M.C., LEHOCKY,M., SOARES,M.R., LAPCIK JR,L., TRINDADE,T.
DYES AND PIGMENTS
2003, 59 (2), PP 181-4.

CLOUD POINTS: CAN WE MEASURE OR MODEL THEM?
HAMMAMI, A., RATULOWSKI, J., COUTINHO, J.A.P.
PETR. SCI. TECH,
2003, 21, PP 345-358.

COMBUSTION SYNTHESIS OF TERNARY CARBIDES OF TI-AL-C SYSTEM
ZHENBIN G.; CHEN K; ZHOU H; NING X AND FERREIRA J M F
J. EUR. CERAM. SOC.
2003, 23, PP 576-574.

COMPARATIVE STUDY OF METALLIC BIOMATERIALS TOXICITY: A HISTOCHEMICAL AND IMMUNOHISTOCHEMICAL DEMONSTRATION IN MOUSE SPLEEN

FERREIRA M E; PEREIRA M L; COSTA F G; SOUSA J P; CARVALHO G S
J. TRACE ELEMENTS IN MED BIOL MED
2003, 17, PP 45-49.

COMPARISON OF DIFFERENT DISPERSANTS PERFORMANCE IN SLIP
CASTING OF CORDIERITE-BASED GLASS-CERAMICS
MEI S; YANG J AND FERREIRA J M F
CERAMICS INTERNATIONAL
2003, 29, PP 785-791.

COMPOSITE GLASS-CERAMICS IN THE SYSTEMS MgO-SiO₂ AND MgO-
Al₂O₃-SiO₂ OBTAINED BY SOL-GEL TECHNOLOGY, B. SAMUNEVA, S.
KALIMANOVA, E. KASHCHIEVA, P. DJAMBASKI, I. M. MIRANDA SALVADO
AND M. H. V. FERNANDES, J. OF SOL-GEL SCIENCE AND TECHNOLOGY
(2003) 26, PP 273-278

CONDUCTIVITY OF CGO AND CSO CERAMICS OBTAINED FROM FREEZE
DRIED PRECURSORS
PEREZ-COLL D, NUÑEZ P, FRADE J R, ABRANTES J C C
ELECTROCHIMICA ACTA
2003, 48, PP 1551-1557

CONTROLLING HYDROLYSIS AND DISPERSING ALN POWDERS IN
AQUEOUS MEDIA
OLIVEIRA M; OLHERO S; ROCHA J AND FERREIRA J M F
J COLL INTERF SCI
2003, 261, PP 456-463.

CRITICAL PHONONS AND IMPURITY Cr³⁺ ZERO-PHONON EMISSION LINE
IN QUANTUM PARAELECTRICS: A- AND B-SITE MG DOPING OF SrTiO₃
TREPAKOV V. A., KUDYK I. B., KAPPHAN S. E., SAVINOV M. E., PASHKIN
A., JASTRABIK L, TKACH A., VILARINHO P. M., KHOLKIN A.L.
JOURNAL OF LUMINESCENCE
2003, 102-103, PP 536-542

CRYSTALCHEMISTRY AND OXIDE ION CONDUCTIVITY IN THE
LANTHANUM OXYGERMANATE APATITE SERIES
LEÓN-REINA L., MARTÍN-SEDEÑO M.C., LOSILLA E.R., CABEZA A.,
MARTÍNEZ-LARA M., BRUQUE S., MARQUES F.M.B., SHEPTYAKOV D. V.,
ARANDA M.A.G.
CHEM. MATER.
2003, 15, PP.2099-2108

CYANIDE-ISOCYANIDE ISOMERS IN POLYNUCLEAR COMPLEXES.
REACTIVITY AND THEORETICAL STUDIES
CALHORDA M J; COSTA P J; DREW M G B; FÉLIX V; GAMELAS C A;
GONÇALVES I S; PEREIRA C C L; ROMÃO C C
INORG. CHIM. ACTA
2003, 356 PP 297-307.

DEPOSITION OF BIOACTIVE GLASS-CERAMIC THIN FILMS BY RF
MAGNETRON SPUTTERING
MARDARE C C; MARDARE A I; FERNANDES J R F; JOANNI E; PINA S C A;
FERNANDES M H V; CORREIA R N
J EUR CERAM SOC
2003, 23, PP 1027-1030

DEGRADATION OF BIPHENYL LIGNIN MODEL COMPOUNDS BY LACCASE
OF *TREMATES VERSICOLOR* IN THE PRESENCE OF 1-
HYDROXYBENZOTRIAZOLE AND HETEROPOLYANION $[SiW_{11}VO_{40}]^{5-}$.
CASTRO A I R.; EVTUGUIN D V; XAVIER A B
J. MOL. CAT. B: ENZYMATIC
2003, 22 (1-2) PP 13-20

DEPOSITION/DETACHMENT OF PARTICLES ON PLASMA TREATED
POLYMER SURFACES
LEHOCKÝ M.; LAPČÍK, JR. L.; NEVES M.C.; TRINDADE T.; SZYK-
WARSZYNSKA, L.; WARSZYNSKI, P.; HUI. D
MATERIALS SCIENCE FORUM
2003, 426-432, PP 2533-2538.

DIELECTRIC PERMITTIVITY AND Cr^{3+} IMPURITY LUMINESCENCE PROBE
OF $Sr_{0.99}Mg_{0.01}TiO_3$ AND $SrTi_{0.99}Mg_{0.01}TiO_3$
TREPAKOV V. A., SAVINOV M. E., KIDYK I. L., PASHKIN A., KAPPAN S. E.,
VILARINHO P. M., TKACH A., KHOLKIN A. L., JASTRABIK L.
FERROELECTRICS
2003, 294, PP 229-238

DIELECTRIC PROPERTIES OF HIGH PRESSURE SYNTHESIZED RELAXOR
 $PbMg_{1/3}Nb_{2/3}O_3$ CERAMICS,
OLEKHNOVICH N M, VYSHATKO N P, RADYUSH Y, SALAK A N, FERREIRA
V M,
J. PHYS.: CONDENS. MATTER,
2003, 15, 6879-87.

DIELECTRIC RELAXATION OF SHALLOW DONOR IN POLYCRYSTALLINE
Mn-DOPED ZnO
HAN J; SENOS A M R; MANTAS PQ; CAO W
J APPL PHYS
2003, 93 (7), PP 4097-4103

DINUCLEAR COPPER AND ZINC COMPLEXES OF A
HEXAAZAMACROCYCLE
CONTAINING *P*-XYLYL SPACERS AND BRIDGING ANIONS: THEORETICAL
AND SPECTROSCOPIC STUDIES
CARVALHO S.; CRUZ C.; DELGADO R., DREW M. G. B. AND FELIX V
DALTON
2003, PP. 4261-4270

DIOXOMOLYBDENUM(VI) MODIFIED MESOPOROUS MCM-41 AND MCM-48 MATERIALS FOR THE CATALYTIC EPOXIDATION OF OLEFINS
NUNES C D; PILLINGER M; VALENTE A A; ROCHA J; LOPES A D;
GONÇALVES I S
EUR J INORG CHEM
2003, PP 3870-3877.

DIRECT OXIDATION OF DRY METHANE ON NANOCRYSTALLINE $CE_{0.8}GD_{0.2}O_{2.8}/PT$ ANODES
YAREMCHENKO A A, VALENTE A A, KHARTON V V, BASHMAKOV I A,
ROCHA J, MARQUES F M B
CATAL COMMUN
2003, 4, PP 477-483.

DOMAIN STRUCTURE, LOCAL HYSTERESIS AND PHASE TRANSITION IN $(CH_3NH_3)_5Bi_2Br_{11}$ (MAPBBB) SINGLE CRYSTALS
WOJTAŚ M., SHVARTSMAN V. V., JAKUBAS R., KHOLKIN A.
FERROELECTRICS
2003, 295, PP 121-129.

EARLY STAGES OF CRYSTALLIZATION OF SOL-GEL DERIVED LEAD ZIRCONATE TITANATE THIN FILMS, CHEM. OF MATER., A. WU, P. M. VILARINHO, I. REANEY, I. M. MIRANDA SALVADO,
2003, 15 (5) 1147-1155.

EASILY DEGRADABLE CHLORINATED COMPOUNDS DERIVED FROM GLUCURONOXILAN IN FILTRATES FROM CHLORINE DIOXIDE BLEACHING OF *EUCALYPTUS GLOBULUS* KRAFT PULP
FREIRE C S R; SILVESTRE A J D; PASCOAL NETO C; SILVA A M S;
EVTUGUIN D V; CAVALEIRO J A S
Holzforschung
2003, 57 (1) PP 81-87

EFFECT OF DISPERSANT ON THE RHEOLOGICAL PROPERTIES AND SLIP CASTING OF CONCENTRATED SIALON PRECURSOR SUSPENSIONS
XU X; OLIVEIRA M I L L; RENLI F AND FERREIRA J M F
J EUROP CERAM SOC
2003, 23, PP 1525-1530.

EFFECT OF IRON DOPING ON THE PROPERTIES OF $TbBaCo_2O_{5.5}$ LAYERED PEROVSKITE
KOPCEWICZ M; KHALYAVIN D D; TROYANCHUK I O; SZYMCZAK H;
SZYMCZAK R; LOGVINOVICH D J; NAUMOVICH E N
J OF APPLIED PHYSIC
2003, 93, PP 479-486

EFFECT OF SOLVENT COMPOSITION ON DISPERSING ABILITY OF REACTION SIALON SUSPENSIONS
XU X; OLIVEIRA M I L L AND FERREIRA J M F
J COLL INTERF SCI

2003, 259, PP 391-397.

EFFECT OF TEXTURE AND MICROSTRUCTURE ON STRAIN HARDENING ANISOTROPY FOR ALUMINUM DEFORMED IN UNIAXIAL TENSION AND SIMPLE SHEAR

LOPES AB, BARLAT F, GRACIO JJ, DUARTE JMF AND RAUCH EF

INT J PLASTICITY

2003, 19 (1), PP 1-22

ELECTRICAL CHARACTERIZATION OF MULLITE/ALUMINA BODIES BASED ON AL-RICH ANODIZING SLUDGE BY IMPEDANCE SPECTROSCOPY

RIBEIRO M J; FERREIRA A A L; FERREIRA J M F AND LABRINCHA J A IONICS

2003, 9, PP 238-241.

ELECTRICAL CONDUCTIVITY OF HEXAGONAL $\text{Ba}(\text{Ti}_{0.94}\text{Ga}_{0.06})\text{O}_{2.97}$ CERAMICS

RAMPLING M.J., MATHER G.C., MARQUES F.M.B., SINCLAIR D.C.

J. EUR. CERAM. SOC.

2003, 23, PP.1911-1917.

ELECTRICAL PROPERTIES OF LITHIUM NIOBIUM SILICATE GLASSES

M.P.F. GRAÇA, M.A. VALENTE e M.G. FERREIRA DA SILVA

J. NON-CRYST. SOLIDS

2003, 325, PP 267-274.

ELECTRON-HOLE TRANSPORT IN $(\text{La}_{0.9}\text{Sr}_{0.1})_{0.98}\text{Ga}_{0.8}\text{Mg}_{0.2}\text{O}_{3-\delta}$

ELECTROLYTE: EFFECTS OF CERAMIC MICROSTRUCTURE

KHARTON V V; SHAULA A L; VYSHATKO N P; MARQUES F M B

ELECTROCHIM ACTA

2003, 48, PP 1817-1828

ELECTRONIC TRANSPORT IN $\text{Ce}_{0.80}\text{Gd}_{0.20}\text{O}_{1.9-\delta}$ UNDER REDUCING CONDITIONS

ABRANTES J C C, PEREZ-COLL D, NUÑEZ P, FRADE, J R

ELECTROCHIMICA ACTA

2003, 48, PP 2761-2766

ENCAPSULATION OF SODIUM NIMESULIDE AND PRECURSORS IN β -CYCLODEXTRIN

BRAGA S S; RIBEIRO-CLARO P; PILLINGER M; GONÇALVES I S; PEREIRA

F; FERNANDES A C; ROMÃO C C; BRITO CORREIA P; TEIXEIRA-DIAS J J C

ORG. BIOMOL. CHEM.

2003, 1 PP 873-878.

ENHANCED EMISSION FROM EU(III) β -DIKETONE COMPLEX COMBINED WITH ETHER-TYPE OXYGEN ATOMS OF DI-UREASIL ORGANIC-INORGANIC HYBRIDS

MOLINA C, DAHMOUCHE K, MESSADDEQ Y, RIBEIRO S J L, SILVA M A P,
BERMUDEZ DE ZEA V, CARLOS L D
J. LUMINESCENCE
2003, 104, PP 93-101

EQUATION OF STATE OF AN ANISOTROPIC THREE-DIMENSIONAL C60
POLYMER: THE MOST STABLE FORM OF FULLERENE
MEZOUAR M; MARQUES L; HODEAU J; NUNEZ-REGEUIRO M
PHYSICAL REVIEW B
2003, 68, PP 193414-193417

EVIDENCE FOR THE AGING OF WAX DEPOSITS IN CRUDE OILS BY
OSTWALD RIPENING
COUTINHO, JAP; DA SILVA, JAL; FERREIRA, A; SOARES, MR; DARIDON, JL
PETROLEUM SCIENCE AND TECHNOLOGY
2003,21 (3-4): PP 381-391

EXTRACTIVE CONTENTS OF TWO WOODS AND CORK OF PORTUGUESE
ORIGIN AND THE INTERACTION OF THESE SUBSTRATES WITH CEMENT
SUSPENSIONS
PEREIRA C; JORGE F C; IRLE M A AND FERREIRA J M F
FOREST PRODUCTS JOURNAL
2003, 53, PP 1-5.

FABRICATION OF ALPHA-SIALON SHEETS BY TAPE CASTING AND
PRESSURELESS SINTERING
XIN X; MEI S AND FERREIRA J M F
JOURNAL OF MATERIALS RESEARCH
2003, 181, PP 363-1367.

FE⁴⁺ FORMATION IN BROWNMILLERITE CAAL_{0.5}FE_{0.5}O_{2.5+δ}
WAARENBORGH J C; ROJAS D P; VYSHATKO N P; SHAULA A L; KHARTON
V V; MAROZAU I P; NAUMOVICH E N
MATER LETT
2003, 57, PP 4388-4393

FRICITION AND WEAR PROPERTIES OF FUNCTIONALLY GRADED
ALUMINUM MATRIX COMPOSITES
GOMES J R; ROCHA L A; CRNKOVIC S J; SILVA R F; MIRANDA A S
MATERIALS SCIENCE FORUM
2003, 423-425, PP 91-96.

FROM POROUS TO COMPACT FILMS BY CHANGING THE ONSET
CONDITIONS OF HW-CVD PROCESS
FERREIRA I; COSTA MEV; FORTUNATO E; MARTINS R
THIN SOLID FILMS
2003, 427, PP 225-230.

GLASS-CERAMICS IN THE FORMER SOVIET UNION: A REVIEW ON
INDUSTRY-ORIENTED DEVELOPMENTS
TULYAGANOV D U; AGATHOPOULOS S; KHARTON V V; MARQUES F M B

IND CERAM

2003, 23, PP 101-115

HALO-DERIVATISED CALIX[4]TUBES

S. E. MATTHEWS; FELIX V.; DREW M. G. B.; BEER P. D.

ORGANIC & BIOMOLECULAR CHEMISTRY

2003, 1(7), PP 1232-1239

HEXENURONIC ACID CONTENTS OF EUCALYPTUS GLOBULUS KRAFT PULPS: VARIATION WITH PULPING CONDITIONS AND EFFECT ON ECF BLEACHABILITY

DANIEL A I.D; PASCOAL NETO C; EVTUGUIN D.V; SILVESTRE A J D TAPPI J.

2003, 2(5) PP 3-8

HIGHLY LUMINESCENT EUROPIUM(III) COMPLEXES WITH NAPHTHOILTRIFLUOROACETONE AND DIMETHYL SULFOXIDE

CARLOS L D, DONEGÁ DE MELLO C, ALBUQUERQUE R Q, ALVES JR S, MENEZES J F S, MALTA O. L.

MOL. PHYS.

2003, 101(7), PP 1037-1045

HISTOLOGY AND HISTOCHEMISTRY IN PLANKTONIC ECOPHYSIOLOGICAL PROCESSES DETERMINATION IN A TEMPERATE ESTUARY (MONDEGO RIVER ESTUARY, PORTUGAL

PASTORINHO M R; ANTUNES C P; MARQUES J C; PEREIRA M L; AZEITEIROU M; MORGADO F M

ACTA OECOLOGICA

2003, 24, PP 235-243.

HOPPING CONDUCTION IN Mn-DOPED ZnO

HAN J; SHEN M; CAO W; SENOS A M R; MANTAS PQ

APPL PHYS LETT

2003, 82 (1), PP 67-69

HOW ALKALI-METAL CATIONS AFFECT THE INCLUSION OF DECANOIC ACID IN β -CYCLODEXTRIN;

LIMA S; GOODFELLOW BJ; TEIXEIRA-DIAS JJC; 2003; 14590-14597;

J.PHYS. CHEM. B.; 107,51.

HYDROTHERMAL SYNTHESIS AND CHARACTERISATION OF TWO NOVEL LARGE-PORE FRAMEWORK VANADIUM SILICATES

BRANDÃO P; VALENTE A A; PHILIPPOU A; FERREIRA A; ANDERSON M W AND ROCHA J

EUR J INORG CHEM

2003, PP 1175-1180.

I-STMAS, A NEW HIGH-RESOLUTION SOLID-STATE NMR METHOD FOR HALF-INTEGER QUADRUPOLAR NUCLEI

AMOUREUX J P ; MORAIS C M; TREBOSC J; ROCHA J AND FERNANDEZ C

SOLID STATE NUCL MAG RESON
2003, 23, PP 213-223.

IMPROVED WEAR RESISTANCE OF SI₃N₄ TOOL INSERTS BY ADDITION OF
AL₂O₃ PLATELETS
OLIVEIRA FJ; SILVA RF AND VIEIRA JM
TRIBOL INT
2003, 36, 1, PP 57-60

IN SITU PREPARATION OF WEAKLY FLOCCULATED AQUEOUS ANATASE
SUSPENSIONS BY THE HYDROTHERMAL TECHNIQUE
YANG J; MEI S AND FERREIRA J M F
J COLL INTERF SCI
2003, 260, PP 82-88.

INFILTRATION OF SIC PREFORMS WITH IRON SILICIDE MELTS:
MICROSTRUCTURES AND PROPERTIES
PAN Y ; GAO MX ; OLIVEIRA FJ; VIEIRA JM AND BAPTISTA JL
MAT SCI ENG A-STRUCT
2003, 359, 1-2, PP 343-349

INFLUENCE OF DEAGGLOMERATION AND CARBOXYL METHYL
CELLULOSE BINDERS ON RHEOLOGICAL BEHAVIOUR OF KAOLIN
SUSPENSIONS
CONCEIÇÃO S I; VELHO J L AND FERREIRA J M F
APP CLAY SCIENCE
2003, 23, PP 257-264.

INFLUENCE OF SHEAR INTENSITY DURING SLIP PREPARATION ON
RHEOLOGICAL CHARACTERISTICS OF CALCIUM CARBONATE
SUSPENSIONS
CONCEIÇÃO S I; OLHERO S; VELHO J L AND FERREIRA J M F
CERAMICS INTERNATIONAL
2003, 29, PP 365-370.

INFLUENCE OF TEMPERATURE ON COLLOIDAL PROCESSING OF
ELECTROSTATICALLY STABILISED ALUMINA SUSPENSIONS
TARÌ G AND FERREIRA J M F
J MATERIALS PROCESSING AND TECHNOLOGY
2003, 137, PP 102-109.

INFLUENCE OF THE DEPOSITION PRESSURE ON THE PROPERTIES OF
TRANSPARENT AND CONDUCTIVE ZNO:GA THIN FILM PRODUCED BY
R.F. SPUTTERING AT ROOM TEMPERATURE
ASSUNÇÃO V; FORTUNATO E; MARQUES A; AGUAS H; FERREIRA I;
COSTA MEV; MARTINS R
THIN SOLID FILMS
2003, 427, PP 401-405.

IONIC TRANSPORT IN $Gd_3Fe_5O_{12}$ - AND $Y_3Fe_5O_{12}$ -BASED GARNETS
KHARTON V V; SHAULA A L; NAUMOVICH E N; VYSHATKO N P;
MAROZAU I P; VISKUP A P; MARQUES F M B
J ELECTROCHEM SOC
2003, 150, PP. J33-42

IN VITRO BIOACTIVITY IN GLASS-CERAMIC / PMMA-CO-EHA
COMPOSITES
FERREIRA B J M L; DUARTE M G G M; GIL M H; CORREIA R N; ROMÁN J;
VALLET-REGÍ M
KEY ENG MATER
2003, 254-256, PP581-584

INORGANIC PLASMA WITH PHYSIOLOGICAL CO_2/HCO_3^- BUFFER
MARQUES, P A A P, MAGALHÃES M C F, CORREIA R N
BIOMATERIALS
2003, 24, PP 1541-1548

INTENSITIES OF $4F-4F$ TRANSITIONS IN GLASS MATERIALS
MALTA O L, CARLOS L D
QUÍMICA NOVA
2003, 26(6), PP 889-895

INTERACTIONS AT THE SURFACE OF OXIDE BIOCERAMICS WITH
BIOLOGICAL LIQUIDS AND AND BLOOD CELLS
AGATHOPOULOS S; CALADO A J; XU J Y; FERRO M C; FERNANDES M H V;
NEDEA M; NIKOLOPOULOS P; CORREIA R N
KEY ENG MATER
2003, 240-242, PP 675-678

INTERACTIONS OF OMEPRAZOLE AND PRECURSORS WITH β -
CYCLODEXTRIN HOST MOLECULES
BRAGA S S; RIBEIRO-CLARO P; PILLINGER M; GONÇALVES I S; A. C.
FERNANDES A C; PEREIRA F; ROMÃO C C; BRITO CORREIA P; TEIXEIRA-
DIAS J J C
J. INCL. PHENOM. MACROCYCLIC CHEM.
2003, 47 PP47-52.

INVESTIGATION OF FERRO-ANTIFERROELECTRIC MIXED STATE IN
TITANIUM MODIFIED $La_{0.03}Sr_{0.255}Ba_{0.7}Nb_2O_6$ FERROELECTRIC CERAMICS
AMORIN,H., PEREZ,J., FUNDORA,A., PORTELLES,J., GUERRERO,F.,
SOARES,M.R., MARTINEZ, E., SIQUEIROS, J.M.
APPL. PHYS. LETT.
2003, 83 (21), PP 4390-4392.

INVESTIGATION OF ORGANIC-INORGANIC HYBRID MATERIALS
PREPARED BY IRRADIATION, A. N. FALCÃO, J. SANTOS SOUSA, I. M.
MIRANDA SALVADO, F. M. A. MARGAÇA, J. TEIXEIRA, L. M. FERREIRA
AND F. G. CARVALHO, J. OF SOL-GEL SCIENCE AND TECHNOLOGY 2003,
26, PP 349-352

INVESTIGATION OF SWITCHING BEHAVIOR IN $\text{PbZr}_{0.45}\text{Ti}_{0.55}\text{O}_3$ THIN FILMS
BY MEANS OF SCANNING PROBE MICROSCOPY

SHVARTSMAN V. V., KHOLKIN A. L.
FERROELECTRICS
2003, 286, PP 291-299

$\text{La}(\text{Mg}_{1/2}\text{Ti}_{1/2})\text{O}_3$ - $\text{La}_{2/3}\text{TiO}_3$ MICROWAVE DIELECTRIC CERAMICS,
SALAK A N, SEABRA M P, FERREIRA V M,
J. EUR. CERAM. SOC.,
2003, 23 (14), PP 2409-2412.

LANTHANIDE COMPLEXES OF 2,6-DIHYDROXYBENZOIC ACID:
SYNTHESIS, CRYSTAL STRUCTURE AND LUMINESCENCE PROPERTIES OF
 $[\text{Bu}_4\text{N}]_2[\text{Ln}(\text{2,6-DHB})_5(\text{H}_2\text{O})_2]$ (Ln = Sm AND Tb)
SOARES-SANTOS P C R; NOGUEIRA H I S; ALMEIDA PAZ F A; SÁ FERREIRA
R A; CARLOS L D; KLINOWSKI J; TRINDADE T
EUR J INORG CHEM
2003, PP 3609-3617.

LANTHANIDE COMPLEXES OF 2-HYDROXYNICOTINIC ACID: SYNTHESIS,
LUMINESCENCE PROPERTIES AND THE CRYSTAL STRUCTURES OF
 $[\text{Ln}(\text{HNICO})_2(\mu\text{-HNICO})(\text{H}_2\text{O})] \cdot n\text{H}_2\text{O}$ (Ln = Tb, Eu)
SOARES-SANTOS P C R; NOGUEIRA H I S; ROCHA J; FÉLIX V; DREW M G B;
SÁ FERREIRA R A; CARLOS L D; TRINDADE T
POLYHEDRON
2003, 22, PP 3529-3539.

LOW INCIDENT ANGLE AND CLASSICAL X-RAY DIFFRACTION ANALYSIS
OF RESIDUAL STRESSES IN DIAMOND COATED Si_3N_4
SOARES, M.R., BELMONTE, M., SILVA, R.F.
J. APPL. PHYS
2003, 94 (9), PP 5633-5638.

MAGNETIC PHASE DIAGRAM FOR A NONEXTENSIVE SYSTEM:
EXPERIMENTAL CONNECTION WITH MANGANITES
REIS M.S., AMARAL V. S., ARAÚJO J. P., OLIVEIRA I.S.
PHYSICAL REVIEW B
2003, 68, PP 010404

MAGNETIC PROPERTIES OF FE-DOPED ORGANIC-INORGANIC
NANOHYBRIDS
SILVA N J O, AMARAL V S, CARLOS L D, BERMUDEZ DE ZEA V
J. APPL. PHYS.
2003, 93(10), PP 6978-6980

MEASUREMENT AND MODELING OF SURFACE TENSIONS OF
ASYMMETRIC SYSTEMS: HEPTANE, EICOSANE, DOCOSANE,
TETRACOSANE AND THEIR MIXTURES

QUEIMADA, A.J., SILVA, F.A.E., CAÇO, A.I., MARRUCHO, I.M., COUTINHO, J.A.P.

FLUID PHASE EQUILIBRIA, 2003, 214, PP 211-221.

MECHANICAL AND ACOUSTIC CHARACTERISTICS OF BOUND RUBBER GRANULATE

SOBRAL M; SAMAGAIO A J B; FERREIRA J M F AND LABRINCHA J A
J MAT PROC TECHN

2003, 142, PP 427-433.

MECHANICALLY-ACTIVATED SYNTHESIS AND MIXED CONDUCTIVITY OF TBMO_{4.8} (M = ZR, HF) CERAMICS

TSIPIS E V; SHLYAKHTINA A V; SHCHERBAKOVA L G; KOLBANEV I V; KHARTON V V; VYSHATKO N P; FRADE J R

J ELECTROCERAM

2003, 10, PP 153-164

METAL COMPLEXES OF A DIPYRIDINE OCTAAZAMACROCYCLE: STABILITY CONSTANTS, STRUCTURAL AND MODELLING STUDIES

CRUZ C; CARVALHO S; DELGADO R; DREW MGB; FELIX V; GOODFELLOW BJ; DALTON TRANSACTIONS;

2003; PP 3172-3183

METAL COMPLEXES OF A TETRAAZACYCLOPHANE: SOLUTION AND MOLECULAR MODELLING STUDIES

ANTUNES; P. P. CAMPELLO M; DELGADO R; DREW M. G. B; FÉLIX V; SANTOS I.

DALTON

2003, PP. 1852-1860

METALLURGICAL SLUDGE IN CLAY-BASED FIRED MATERIALS

COUTO D M; RINGUEDÉ A; SILVA R F; LABRINCHA J A; RODRIGUES C M S
CERAM BULL

2003, 82, PP 9101-9103.

MICROPOROUS MATERIALS CONTAINING LANTHANIDE METALS

ROCHA J AND CARLOS L D

CURR OPIN SOLID STATE MATER SCI

2003, 7, PP 199-205.

MICROSTRUCTURE AND LOCAL PIEZOELECTRIC PROPERTIES OF (Pb,Ca)TiO₃ THIN FILMS

SHVARTSMAN V. V., CALZADA M. L., POYATO R., PARDO L., KHOLKIN A. L., FERROELECTRICS

2003, 296, PP 229-237

MINERALIZATION OF TWO CALCIUM PHOSPHATE CERAMICS IN BIOLOGICAL MODEL FLUID

MARQUES, P A A P, SERRO A P, SARAMAGO B J, FERNANDES A C, MAGALHÃES M C F, CORREIA R N

J MAT CHEM
2003, 13, PP 1484-1490

MINERALIZATION OF TWO PHOSPHATE CERAMICS IN HBSS: ROLE OF ALBUMIN

MARQUES, P A A P, SERRO A P, SARAMAGO B J, FERNANDES A C,
MAGALHÃES M C F, CORREIA R N
BIOMATERIALS
2003, 13, PP 451-460

MOLECULAR STRUCTURE-ACTIVITY RELATIONSHIPS FOR THE OXIDATION OF ORGANIC COMPOUNDS USING MESOPOROUS SILICA CATALYSTS DERIVATISED WITH BIS(HALOGENO) DIOXOMOLYBDENUM(VI) COMPLEXES

NUNES C, VALENTE A A, PILLINGER M, ROCHA J, GONÇALVES I S
CHEM EUR. J
2003, 9, PP 4380-4390

MONO- AND BINUCLEAR BIPYRIDYL DERIVATIVES OF THE $MO(\eta^3-C_3H_5)(CO)_2$

FRAGMENT: STRUCTURAL STUDIES AND FLUXIONALITY IN SOLUTION
COSTA P. M.F.J.; MORA M.; CALHORDA M. J.; FELIX V, FERREIRA P. DREW M.G.B.; W.HUBERT;
JOURNAL OF ORGANOMETALLIC CHEMISTRY
2003, 687, PP 57-68

MONOTERPENES OXIDATION IN THE PRESENCE OF Y ZEOLITE-ENTRAPPED MANGANESE(III) TETRA(4-N-BENZYLPIRIDYL)PORPHYRIN
SKROBOT F C, VALENTE A A, NEVES G, ROSA I, ROCHA J, CAVALEIRO J A S

J MOL CATAL A-CHEM
2003, 201, PP 211-222.

MULLITE-ALUMINA REFRACTORY CERAMICS OBTAINED FROM MIXTURES OF NATURAL COMMON MATERIALS AND RECYCLED AL-RICH ANODIZING SLUDGE

TULYAGANOV D U; OLHERO S; RIBEIRO M J; LABRINCHA J A AND FERREIRA J M F
JOURNAL OF MATERIALS SYNTHESIS AND PROCESSING
2003, 10, PP 313-318.

NANOSCALE DOMAINS AND LOCAL PIEZOELECTRIC HYSTERESIS IN $PB(Zn_{1/3}Nb_{2/3})O_3-4.5\%PbTiO_3$ SINGLE CRYSTALS

BDIKIN I. K., SHVARTSMAN V. V., KHOLKIN A. L.
APPLIED PHYSICS LETTERS
2003, 83, PP 4232-4234

NITRATE OCCLUSION STUDIES IN Y ZEOLITE AND IN A CLAY PILLARED WITH ALUMINIUM OXIDE

CARVALHO A; PIRES J; VELOSO P; MACHADO M; BROTAS DE CARVALHO M AND ROCHA J
MICROPOROUS MESOPOROUS MATER
2003, 58, PP 163-173

NMR SOLUTION STRUCTURES OF TWO MUTANTS OF DESULFOREDOXIN;
GOODFELLOW BJ; RUSNAK F; MOURA I; ASCENSO CS; MOURA JJG;
JOURNAL OF INORGANIC BIOCHEMISTRY; 93, 1-2
2003; PP 100-108

NOVEL LANTHANIDE LUMINESCENT MATERIALS BASED ON
COMPLEXES OF 3-HYDROXYPICOLINIC ACID AND SILICA
NANOPARTICLES
SOARES-SANTOS P C R; NOGUEIRA H I S; FÉLIX V; DREW M G B; SÁ
FERREIRA R A; CARLOS L D; TRINDADE T
CHEM MATER
2003, 15, PP 100-108.

NOVEL NUCLEAR MAGNETIC RESONANCE TECHNIQUES FOR THE STUDY
OF QUADRUPOLAR NUCLEI IN CLAYS AND OTHER LAYERED MATERIALS
ROCHA J; MORAIS C M AND FERNANDEZ C
CLAY MIN
2003, 38, PP 259-278.

ON THE HALF UNIT CELL INTERGROWTH OF $\text{Bi}_2\text{Sr}_2\text{Ca}_3\text{Cu}_4\text{O}_x$ WITH OTHER
SUPERCONDUCTING PHASES IN TWO-STEP ANNEALED LFZ FIBERS
YANG L; COSTA F M; LOPES A B; SILVA R F; VIEIRA J M
PHYSICA C
2003, 398, PP 31-36.

ON THE RELATIONSHIPS BETWEEN STRUCTURE, OXYGEN
STOICHIOMETRY AND IONIC CONDUCTIVITY OF $\text{CaTi}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$ ($X = 0.05,$
 $0.20, 0.40, 0.60$)
FIGUEIREDO F M; WAERENBORGH J C; KHARTON V V; NAEFE H; FRADE J
R
SOLID STATE IONICS
2003, 156, PP 371-381

ORDERED BENZENE-SILICA HYBRIDS WITH MOLECULAR-SCALE
PERIODICITY IN THE WALLS AND DIFFERENT MESOPORE SIZES
BION N; FERREIRA P; VALENTE A A; GONÇALVES I S; ROCHA J
J. MATER. CHEM.
2003, 13 PP1910-1913.

ORDERING MECHANISM IN HIGH-PRESSURE POLYMERIZATION OF
C60: AVOIDING GEOMETRICAL FRUSTRATION BY STRESS-DRIVEN BOND
SELECTION
MARQUES L; MEZOUAR M; HODEAU J; NUNEZ-REGUEIRO M
PHYSICAL REVIEW B
2003, 68, PP193408-193411

OXIDATION OF DRY METHANE ON THE SURFACE OF OXYGEN ION-CONDUCTING MEMBRANES

YAREMCHENKO A A, VALENTE A A, KHARTON V V, TSIPIE E V, FRADE J R, NAUMOVICH E N, ROCHA J, MARQUES F M B

CATAL LETT

2003, 91, PP 169-174.

OXIDATION OF MONOTERPENES WITH HYDROGEN PEROXIDE CATALYSED BY KEGGIN-TYPE TUNGSTOBORATES

SANTOS, I C M S; SIMÕES, M M Q; PEREIRA, M M M S; MARTINS, R R L;

NEVES, M G P M S; CAVALEIRO, J A S; CAVALEIRO, A M V

J. MOL. CATAL. A- CHEMICAL

2003, 195, PP 253-262.

OXIDATION OF PINANE OVER PHTHALOCYANINE COMPLEXES SUPPORTED ON ACTIVATED CARBON. EFFECT OF THE SUPPORT SURFACE TREATMENT

VALENTE A, PALMA C, FONSECA I M, RAMOS A M, VITAL J

CARBON

2003, 41, PP 2793-2803

OXIDISED DERIVATIVES OF LIPOPHILIC EXTRACTIVES FORMED DURING HARDWOOD KRAFT PULP BLEACHING.

FREIRE C S R.; SILVESTRE A J D AND NETO C P

HOLZFORSCHUNG

2003, 57(5) PP 503-512

OXYGEN BLEACHING OF KRAFT PULP CATALYSED BY MN(III)-SUBSTITUTED POLYOXOMETALATES

GASPAR A; EVTUGUIN D V; PASCOAL NETO C

APPLIED CAT A: GENERAL

2003, 239 (1-2) PP 157-168

OXYGEN DEFICIENCY AND PHASE TRANSITIONS IN $\text{SrCO}_{1-x-y}\text{Fe}_x\text{Cr}_y\text{O}_{3-\delta}$ (X = 0.10-0.40, Y = 0-0.05)

TIKHONOVICH V N; NAUMOVICH E N; LOGVINOVICH D I; KHARTON V V; VECHER A A

J SOLID STATE ELECTROCHEM

2003, 7, PP 77-82

OXYGEN IONIC AND ELECTRONIC TRANSPORT IN $\text{Gd}_{2-x}\text{Ca}_x\text{Ti}_2\text{O}_{7-\delta}$ PYROCHLORES

KHARTON V V; TSIPIE E V; YAREMCHENKO A A; VYSHATKO N P; SHAULA A L; NAUMOVICH E N; FRADE J R

J SOLID STATE ELECTROCHEM

2003, 7, PP 468-476

OXYGEN IONIC CONDUCTION IN BROWNMILLERITE $\text{CaAl}_{0.5}\text{Fe}_{0.5}\text{O}_{2.5+\delta}$

KHARTON V V; MAROZAU I P; VYSHATKO N P; SHAULA A L; VISKUP A P;
NAUMOVICH E N; MARQUES F M B
MATER RES BULL
2003, 38, PP 773-782

OXYGEN IONIC CONDUCTIVITY OF PEROVSKITE-TYPE $LA_{1-x}SR_xGA_{1-y}MG_yM_{0.20}O_{3-\delta}$ (M = FE, CO, NI)
YAREMCHENKO AA; SHAULA A L; LOGVINOVICH D I; KHARTON V V;
KOVALEVSKY A V; NAUMOVICH E N; FRADE J R; MARQUES F M B
MATER CHEM PHYS
2003, 82, PP 684-690

OXYGEN NONSTOICHIOMETRY OF $SR(CO,FE)O_{3-\delta}$ -BASED PEROVSKITES. I.
COULOMETRIC TITRATION OF $SRCO_{0.85}FE_{0.10}CR_{0.05}O_{3-\delta}$ BY THE TWO-
ELECTRODE TECHNIQUE
TIKHONOVICH V N; ZHARKOVSKAYA O M; NAUMOVICH E N;
BASHMAKOV I A; KHARTON V V; VECHER A A
SOLID STATE IONICS
2003, 160, PP 259-270

OXYGEN PERMEABILITY OF PEROVSKITE-TYPE $SR_{0.7}CE_{0.3}MNO_{3-\delta}$
KHARTON V V; VISKUP A P; MAROZAU I P; NAUMOVICH E N
MATER LETT
2003, 57, PP 3017-3021

OXYGEN PERMEABILITY OF $LAGAO_3$ -BASED CERAMIC MEMBRANES
SHAULA A L; YAREMCHENKO A A; KHARTON V V; LOGVINOVICH D I;
NAUMOVICH E N; KOVALEVSKY A V; FRADE J R; MARQUES F M B
J MEMBRANE SCI
2003, 221, PP 69-77

OXYGEN PERMEABILITY OF $LAGA_{0.65}NI_{0.20}MG_{0.15}O_{3-\delta}$ CERAMICS: EFFECT
OF SYNTHESIS METHOD
SHAULA A L; VISKUP A P; KHARTON V V; LOGVINOVICH D I;
NAUMOVICH E N; FRADE J R; MARQUES F M B
MATER RES BULL
2003, 38, PP 353-362

OXYGEN TRANSPORT IN $CE_{0.8}GD_{0.2}O_{2-\delta}$ - BASED COMPOSITE MEMBRANES
KHARTON V V; KOVALEVSKY A V; VISKUP A P; SHAULA A L;
FIGUEIREDO F M; NAUMOVICH E N; MARQUES F M B
SOLID STATE IONICS
2003, 160, PP 247-258

P-TYPE ELECTRONIC CONDUCTIVITY, OXYGEN PERMEABILITY AND
STABILITY OF $LA_2NI_{0.9}CO_{0.1}O_{4+\delta}$
YAREMCHENKO A A, KHARTON V V, PATRAKEEV M V, FRADE J R
J. MAT. CHEM.
13, 2003, PP 1136-1149.

P-TYPE ELECTRONIC TRANSPORT IN $\text{Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{2-\delta}$: THE EFFECT OF
TRANSITION METAL OXIDE SINTERING AIDS

FAGG D P; KHARTON V V; FRADE J R

J ELECTROCERAM

2002, 9, PP 199-207.

(PUBLISHED FEBRUARY 2003)

PLASMA SURFACE MODIFICATION OF POLYETHYLENE

LEHOCKÝ M; DRNOVSKÁ H; LAPCIKOVÁ B; BARROS-TIMMONS A;

TRINDADE T; ZEMBALA M; AND LAPCIK, JR L

COLLOID AND SURFACES A

2003, 222 (1-3), PP 125-131

PLASTIC FLOW FOR NON-MONOTONIC LOADING CONDITIONS OF AN
ALUMINUM ALLOY SHEET SAMPLE

BARLAT F, DUARTE JMF, GRACIO JJ, LOPES AB AND RAUCH EF.

INT J PLASTICITY

2003, 19 (8), PP1215-1244

POLYMORPHISM IN TETRABUTYLAMMONIUM SALTS OF KEGGIN-TYPE
POLYOXOTUNGSTATES

GAMELAS, J. A F; SOARES, M R; FERREIRA, A; CAVALEIRO, A M V

INORG. CHIMICA ACTA

2003, 342, PP 16-22.

POWDER X-RAY DIFFRACTION STUDY OF $\text{LaCo}_{0.5}\text{Ni}_{0.5}\text{O}_{3-\delta}$ AND
 $\text{LaCo}_{0.5}\text{Fe}_{0.5}\text{O}_{3-\delta}$

VYSHATKO N P; KHARTON V V; SHAULA A L; MARQUES F M B

POWDER DIFFR

2003, 18, PP 159-161

PREPARATION AND CATALYTIC PROPERTIES OF A NEW
DIOXOMOLYBDENUM(VI) COMPLEX COVALENTLY ANCHORED TO
MESOPOROUS MCM-48

NUNES C D; PILLINGER M; VALENTE A A; ROCHA J; LOPES A D;

GONÇALVES I S

INORG CHEM COMMUN

2003, 6, PP 1228-1233.

PREPARATION AND CHARACTERISATION OF ORGANOTIN-
OXOMOLYBDATE COORDINATION POLYMERS AND THEIR USE IN
SULFOXIDATION CATALYSIS

ABRANTES M, VALENTE A A, PILLINGER M, GONÇALVES I S, ROCHA J,
ROMÃO C C

CHEM EUR J

2003, 9, PP 2685-2695.

PREPARATION OF HOLLOW SHELLS OF ZINC OXIDE/BISMUTH (III)

VANADATE NEVES M. C.; TRINDADE T.

MATER. RES. BULL.

2003, 38, PP 1013-1020.

PREPARATION OF HOMOGENEOUS REACTION SIALON SUSPENSIONS FOR SLIP CASTING

XIN X; OLIVEIRA M I L L AND FERREIRA J M F

MATERIALS SCIENCE FORUM

2003, 442-442, PP 103-108.

PROCESSING AND DIELECTRIC PROPERTIES OF $\text{La}(\text{Mg}_{0.5}\text{Ti}_{0.5})\text{O}_3\text{-BaTiO}_3$ CERAMICS,

SEABRA M P, SALAK A N, FERREIRA V M, VIEIRA L G, RIBEIRO J L, FERROELECTRICS,

2003,294, PP 165-173.

PULSED LASER ANNEALING OF SI-GE SUPERLATTICES

SOBOLEV NA, IVLEV GD, GATSKEVICH EI, LEITÃO JP, FONSECA A.,

CARMO MC, LOPES AB, SHARAEV DN, KIBBEL H, PRESTING H.

MAT SCI ENG C

2003, 23 (1-2), PP 19-22

RAMAN SPECTROSCOPY AND PYROELECTRIC STUDIES OF SrTiO_3 CERAMICS DOPED WITH DIFFERENT CONCENTRATIONS OF BISMUTH

A. ALMEIDA, PEDRO TELES, M. R. CHAVES, P. M. VILARINHO, J. L.

BAPTISTA

FERROELECTRICS

2003, 294, PP 49/[405] – 60/[416].

RAMAN STUDIES OF THE FE-AFE PHASE TRANSITION IN CERAMIC

$\text{Li}_{0.12}\text{Na}_{0.88}\text{Ta}_{0.2}\text{Nb}_{0.8}\text{O}_3$ SOLID SOLUTION

SIDOROV N. V., PALATNIKOV M. N., GOLUBYATNIK N. A., BORMANIS K.,

KHOLKIN A., STERNBERG A.

FERROELECTRICS

2003, 294, PP 221-227

REDOX BEHAVIOUR OF $\text{Sr}_4\text{Fe}_6\text{O}_{13\pm\delta}$ BY MÖSSBAUER SPECTROSCOPY AND NEUTRON DIFFRACTION

WAERENBORGH J C; AVDEEV M; PATRAKEEV M V; KHARTON V V; FRADE J R

MATER LETT

2003, 57, PP 3245-3250

RELAXOR BEHAVIOR OF $\text{BaBi}_2\text{Ta}_2\text{O}_9$ AND $\text{BaBi}_2\text{Nb}_2\text{O}_9$ CERAMICS

SHVARTSMAN V. V., COSTA M. E. V., AVDEEV M., KHOLKIN A. L.

FERROELECTRICS

2003, 296, PP 187-197

RHEOLOGICAL BEHAVIOUR OF CLAY-BASED SLURRIES: EFFECT OF THE PREPARATION METHODS (LAB-SCALE OR TYPICAL INDUSTRIAL PROCEDURES)

PEREIRA F R; OLIVEIRA A P; DE NONI JR. A; HOTZA D; SEGADÃES A M;
LABRINCHA J A
INDUSTRIAL CERAMICS
2003, 23 [2] PP 87-92

ROOM TEMPERATURE VISIBLE/INFRARED EMISSION AND ENERGY
TRANSFER IN Nd^{3+} -BASED ORGANIC/INORGANIC NANOHYBRIDS
SÁ FERREIRA R A, CARLOS L D, BERMUDEZ DE ZEA V, MOLINA C,
DAHMOUCHE K, MESSADDEQ Y, RIBEIRO S J L
J. SOL-GEL SCI. TECH
2003, 26(1-3), PP 315-319

SANS STUDY OF ZIRCONIA-SILICA AND TITANIA-SILICA HYBRID
MATERIALS, A. N. FALCÃO, J. SANTOS SOUSA, I. M. MIRANDA SALVADO,
F. M. A. MARGAÇA, J. TEIXEIRA AND F. G. CARVALHO, J. OF SOL-GEL
SCIENCE AND TECHNOLOGY (2003) 26, PP 345-348

SEGMENTATION AND MORPHOMETRY OF HISTOLOGICAL SECTIONS
USING DEFORMABLE MODELS: A NEW TOOL FOR EVALUATING
TESTICULAR HISTOPATHOLOGY
GUEVARA M; SILVA A; OLIVEIRA H; PEREIRA M L; MORGADO F
LECTURE NOTES ON COMPUTER SCIENCES
2003, 2905, PP 282-290.

SHORT-CHAIN DI-UREASIL ORMOLYTES DOPED WITH POTASSIUM
TRIFLATE: PHASE DIAGRAM AND CONDUCTIVITY BEHAVIOR
BERMUDEZ DE ZEA V, GOMES CORREIA S M, SILVA M M, BARROS S,
SMITH M J, SÁ FERREIRA R A, CARLOS L D, MOLINA C, RIBEIRO S J L
J. SOL-GEL SCI. TECH
2003, 26(1-3), PP 375-381

SINTERING OF TUNGSTEN CARBIDE PARTICLES SPUTTER-DEPOSITED
WITH STAINLESS STEEL
FERNANDES C M; SENOS A M R; VIEIRA, M T
INT J REF MET & HARD MAT
2003, 21, PP 147-154

Si_3N_4 AND $\text{Si}_3\text{N}_4/\text{SiC}$ COMPOSITE RINGS FOR DYNAMIC SEALING OF
CIRCULATING FLUIDS
CARRAPICHANO JM; GOMES JR; OLIVEIRA FJ AND SILVA RF
WEAR
2003, 255, PP 695-698

SMALL-ANGLE X-RAY SCATTERING AND X-RAY ABSORPTION NEAR-
EDGE STRUCTURE STUDY OF IRON-DOPED SILOXANE-
POLYOXYETHYLENE NANOCOMPOSITES
CHIAVACCI L A, DAHMOUCHE K, SANTILLI C V, BERMUDEZ DE ZEA V,
CARLOS L D, BRIOIS V, CRAIEVICH A F
J. APPL. CRYSTALLOGR.
2003, 36, PP 405-409

SOL-GEL DERIVED FLUORINATED HYDROXYAPATITE FILMS
CHENG K; HAN G; WENG W; QU H; DU P; SHEN G; YANG J AND FERREIRA
J M F

MATERIAL RESEARCH BULLETIN
2003, 38, PP 89-97.

SOL-GEL DERIVED POE/SILICEOUS HYBRIDS DOPED WITH Na^+ IONS:
MORPHOLOGY AND IONIC CONDUCTIVITY
GOMES CORREIA S M, BERMUDEZ DE ZEA V, SILVA M M, BARROS S, SÁ
FERREIRA R A, CARLOS L D, PASSOS DE ALMEIDA A P, SMITH M J

SOLID STATE IONICS
2003, 156(1-2), PP 85-93

SOL-GEL PREPARATION AND PRELIMINARY *IN VITRO* EVALUATION OF
FLUORAPATITE/HYDROXYAPATITE SOLID SOLUTION FILMS
WENJIAN W; CHENLU S; CHENG K; HAIBO Q; PIYI D, SHEN G; GAORONG
H; YANG J AND FERREIRA J M F

J MATER SCI TECHNOL
2003, 19, PP 495-498.

SOLID STATE INCLUSION COMPOUND OF S-IBUPROFEN IN β -
CYCLODEXTRIN: STRUCTURE AND CHARACTERIZATION
BRAGA S S; GONÇALVES I S; HERDTWECK E; TEIXEIRA-DIAS J J C

NEW J. CHEM.
2003, 27 PP 597-601

SOLUBILITY OF OXYGEN IN HEXANE AND PERFLUOROHEXANE:
EXPERIMENTS AND SIMULATION

DIAS A.M., MARRUCHO I.M., PADUA A.A., COSTA GOMES M.,
PCCP
2003, 5(3), PP 543

SPERMATOGENESIS RECOVERY IN THE MOUSE AFTER IRON INJURY
PEREIRA M L; COSTA F G;

Human Exp Toxicol
2003, 22, PP 275-279.

STABILITY AND MIXED IONIC-ELECTRONIC CONDUCTIVITY OF
(SR,LA)(TI,FE) $\text{O}_{3-\delta}$ PEROVSKITES

FAGG D P, KHARTON V V, FRADE J R, FERREIRA A A L
SOLID STATE IONICS
2003, 156, PP 45-57

STABILITY AND OXYGEN IONIC CONDUCTIVITY OF ZIRCON-TYPE $\text{Ce}_{1-x}\text{A}_x\text{VO}_{4+\delta}$ (A = CA, SR)

TSIPIS E V, KHARTON V V, VYSHATKO N P, SHAULA A L, FRADE J R
J. SOLID STATE CHEM.
2003, 176, PP 47-56

STABILITY OF LEAD(II) ARSENATES
MAGALHÃES M C F, SILVA MCM
MONATSCHEFTE FÜR CHEMIE
2003, 134, PP 735-743

STAINLESS STEEL COATINGS SPUTTER-DEPOSITED ON TUNGSTEN
CARBIDE POWDER PARTICLES
FERNANDES C M; FERREIRA V M; SENOS A M R; VIEIRA, M T
SURF COATINGS TECHN
2003, 176, PP 103-108

STRONG EXPERIMENTAL EVIDENCE OF C-H...O HYDROGEN BONDS IN
CYCLOPENTANONE:
THE SPLITTING OF THE NC=O MODE REVISITED
VAZ P D; RIBEIRO-CLARO P J A
J. PHYS. CHEM. A, 2003, 107, 6301-6305

STRUCTURAL AND ELECTRICAL PROPERTIES OF IRON-CONTAINING
ALUMINOSILICATE GEL-DERIVED PELLETS
M.G. FERREIRA DA SILVA e M.A. VALENTE
J. SOL-GEL SCI. TECHNOL..
2003, 26, PP 1091- 1096

STRUCTURE AND DIELECTRIC CHARACTERIZATION OF $\text{La}(\text{Mg}_{1/2}\text{Ti}_{1/2})\text{O}_3$ -
 $\text{Nd}(\text{Mg}_{1/2}\text{Ti}_{1/2})\text{O}_3$ SYSTEM,
SEABRA M P, SALAK A N, AVDEEV M, FERREIRA V M,
J. PHYS.: CONDENS. MATTER,
2003,15 (24), PP 4229-4238.

STRUCTURE AND MICROWAVE DIELECTRIC PROPERTIES OF
 $\text{La}(\text{Mg}_{0.5}\text{Ti}_{0.5})\text{O}_3$ - CaTiO_3 SYSTEM,
SEABRA M P, AVDEEV M, FERREIRA V M, PULLAR R C, ALFORD N,
J. EUR. CERAM. SOC.,
2003, 23 (14), PP 2403-2408.

STRUCTURE OF LUMINESCENT MONO AND DI-URETHANESILS
NANOCOMPOSITES DOPED WITH Eu^{3+} IONS
DAHMOUCHE K, GONÇALVES M C, SANTILLI C V, BERMUDEZ DE ZEA V,
CARLOS L D, CRAIEVICH A F
NUCL. INSTRUM. METHODS PHYS. RES. SECT. B
2003, 199, PP 117-122

STRUCTURE OF LUMINESCENT MONO AND DI-URETHANESILS
NANOCOMPOSITES DOPED WITH Eu^{3+} IONS
DAHMOUCHE K, GONÇALVES M C, SANTILLI C V, BERMUDEZ DE ZEA V,
CARLOS L D, CRAIEVICH A F
NUCL. INSTRUM. METHODS PHYS. RES. SECT. B
2003, 211, PP 160-160

STRUCTURE OF MAGNETIC POE-SILOXANE NANOHYBRIDS WITH FE(II) AND FE(III)

SILVA N J O, AMARAL V S, CARLOS L D, DAHMOUCHE K, SANTILLI C V,
BERMUDEZ DE ZEA V, CRAIEVICH A F
J. APPL. CRYSTALLOGR.
2003, 36(4), PP 961–966

STRUCTURE TRANSFORMATIONS AND DIELECTRIC PROPERTIES OF
 $\text{PbY}_{1/2}\text{Nb}_{1/2}\text{O}_3$ AND $\text{PbHo}_{1/2}\text{Nb}_{1/2}$ COMPOUNDS,
SALAK A N, VYSHATKO N P, FERREIRA V M, OLEKHNOVICH N M, SHILIN
A D,
MATERIALS RESEARCH BULLETIN,
2003, 38 (3), PP 453-460

SUBMILLIMETER AND FAR INFRARED DIELECTRIC RESPONSE OF BI-
DOPED SrTiO_3 CERAMICS
ALEXEJ PASHKIN, POLINA SAMOUKHINA, TETYANA OSTAPCHUK,
PETR KUZEL, PAULA VILARINHO, AND JAN PETZELT
FERROELECTRICS
2003, 294, PP 133/[489] – 140[496].

SYNTHESIS AND ASSEMBLY OF SiO_2 COATED Bi_2S_3 NANOFIBERS
NEVES M. C.; LIZ-MARZÁN L. M.; TRINDADE T.
J. COLLOID INTERFACE SCI.
2003, 264, PP 391-395

SYNTHESIS AND CHARACTERISATION OF CERMET ANODES FOR SOFCs
WITH A PROTON-CONDUCTING CERAMIC PHASE
MATHER G C, FIGUEIREDO F M, JURADO J R, FRADE J R
SOLID STATE IONICS
2003, 162, PP 115-120

SYNTHESIS AND CHARACTERISATION OF LEAD ZIRCONATE TITANATE
FIBERS PREPARED BY SOL-GEL METHOD: THE ROLE OF THE ACID, MEI
ZHANG, I. M. MIRANDA SALVADO, PAULA M. VILARINHO, J. OF AMER.
CERAMIC SOC., (2003) 86, 5, PP 775-81

SYNTHESIS AND CHARACTERIZATION OF $\text{Ni-SrCe}_{0.9}\text{Yb}_{0.1}\text{O}_{3-\delta}$ CERMET
ANODES FOR PROTONIC CERAMIC FUEL CELLS
MATHER G C, FIGUEIREDO F M, FAGG D P, NORBY T, JURADO J R, FRADE
J R
SOLID STATE IONICS
2003, 158, PP 333-342

SYNTHESIS AND CHARACTERIZATION OF $\text{SrBi}_2\text{Ta}_2\text{O}_9$ POWDERS FOR
FERROELECTRIC APPLICATIONS
AGUILAR GG; COSTA MEV
FERROELECTRICS
2003, 294, PP 211-220.

SYNTHESIS AND LUMINESCENCE OF Eu^{3+} -DOPED NARSARSUKITE
PREPARED BY THE SOL-GEL PROCESS

RAINHO J P; LIN Z; ROCHA J AND CARLOS L D
J. SOL-GEL SCI TECHNOL
2003, 26, PP 1005-1009.

SYNTHESIS AND STRUCTURAL CHARACTERISATION OF NOVEL TIN AND
TITANIUM POTASSIUM SILICATES $K_4M_2Si_6O_{18}$
LIN Z; FERREIRA A AND ROCHA J
J SOLID STATE CHEM
2003, 175, PP 258-263.

STRESS-INDUCED SUPPRESSION OF PIEZOELECTRIC PROPERTIES IN
PbTiO₃:La THIN FILMS VIA SCANNING FORCE MICROSCOPY
KHOLKIN A. L., SHVARTSMAN V. V., EMEL'YANOV A. YU., POYATO R.,
PARDO L. APPLIED PHYSICS LETTERS
2003, 82, PP 2127-229

STRUCTURAL AND MECHANICAL CHARACTERISATION OF MGO-, CAO-,
AND BAO-DOPED ALUMINOSILICATE CERAMICS
OLIVEIRA M AND FERREIRA J M F
MAT. SCI. & ENG.
2003, A344, PP 35-44.

STRUCTURAL CHARACTERISATION AND DFT STUDIES OF
[CR(CYCLAM)(O-DMSO)CL]²⁺: A NEW PRECURSOR COMPLEX TOWARDS
POTENTIAL DNA INTERCALATORS;
FÉLIX V; SANTOS TM; MADUREIRA J; MIRANTE F; QUINTAL S;
GOODFELLOW BJ; SANTANA-MARQUES MG; PEDROSA DE JESUS J; DREW
MGB; CALHORDA MJ;
2003;; INORG. CHIM. ACTA.; 356. PP 335-342

STRUCTURAL CHARACTERIZATION OF MIXED CONDUCTING
PEROVSKITES LA(GA,M)O_{3-δ} (M = MN, FE, CO, NI)
VYSHATKO N P; KHARTON V V; SHAULA A L; NAUMOVICH E N;
MARQUES F M B
MATER RES BULL
2003, 38, PP 185-193

STRUCTURAL INTERPRETATION OF THE IN VITRO REACTIVITY OF SiO₂-
MGO-NA₂O GLASSES
AGATHOPOULOS S; XU J Y; FERRO M C; FERNANDES M H V; OLIVEIRA J
M; MARQUES PAAP; CORREIA R N
KEY ENG MATER
2003, 240-242, PP 217-220

STRUCTURE ANALYSIS OF THE NOVEL MICROPOROUS
ALUMINOPHOSPHATE IST-1 USING SYNCHROTON POWDER DIFFRACTION
DATA AND HETCOR MAS NMR
JORDÁ J L; MCCUSKER L B; BAERLOCHER C; MORAIS C M; ROCHA J;
FERNANDEZ C; BORGES C; LOURENÇO J P; RIBEIRO M F AND GABELICA Z
MICROPOROUS MESOPOROUS MAT

2003, 65, PP 43-57.

STUDY OF CATALYST SELECTIVITY IN THE OXIDATION OF PHENOL

ROCHA G O; ROCHA J AND LIN Z

CATAL LETT

2003, 89, PP 69-74.

STUDY OF INERTIZATION REACTIONS OF METAL PLATING SLUDGES IN
CLAY-BASED MATERIALS BY IMPEDANCE SPECTROSCOPY

COUTO D M S; RODRIGUES C M S; SILVA R F; LABRINCHA J A

AMER. CERAM. SOC. BULL (ON-LINE VERSION)

2003, 12, PP 911-913.

SUITABILITY OF PZT CERAMICS FOR MASS SENSORS VERSUS

WIDESPREAD USED QUARTZ CRYSTALS

VERISSIMO M I S; SENOS A M R; MANTAS PQ; OLIVEIRA J A B P; GOMES

M T S R

SENSORS AND ACTUATORS-B, 2003, 95, PP 25-31

SURFACE ADSORPTION OF 4,4'-DITHIODIPYRIDINE AND 2,2'-

DITHIODIPYRIDINE ON SILVER NANOPARTICLES

NOGUEIRA H I S; CRUZ S M G; SOARES-SANTOS P C R; RIBEIRO-CLARO P

J; TRINDADE T

J RAMAN SPECTROSC

2003, 34, PP 350-356.

SURFACE PRETREATMENTS OF SILICON NITRIDE FOR CVD DIAMOND DEPOSITION

BELMONTE M; SILVA V A; FERNANDES A J S; COSTA F M; SILVA R F

J AMER CERAM SOC

2003, 86, PP 749-754.

SURFACE PROPERTIES OF POLYETHYLENE AFTER LOW-TEMPERATURE
PLASMA TREATMENT

DRNOVSKÁ H; LAPCIK, JR L; BURSIKOVÁ V; ZEMEK J AND BARROS-

TIMMONS A

COLLOID POLYMER SCI.

2003, 281 (11), PP 1025-1033.

SYNTHESIS AND CRYSTAL STRUCTURE OF $[\text{Bu}_4\text{N}][\text{Er}(\text{PIC})_4] \cdot 5.5\text{H}_2\text{O}$: A
NEW INFRARED EMITTER

SOARES-SANTOS P C R; NOGUEIRA H I S; FÉLIX V; DREW M G B; SÁ

FERREIRA R A; CARLOS L D; TRINDADE T

INORG CHEM COM

2003, 6, PP 1234-1238.

SYNTHESIS AND DIELECTRIC PROPERTIES OF TUNGSTEN-BASED
COMPLEX PEROVSKITES

KHALYAVIN D D; HAN J; SENOS A M R; MANTAS PQ

J MAT RES

2003, 18 (11), PP 2600-2607

SYNTHESIS AND STRUCTURAL CHARACTERISATION OF NOVEL TIN AND TITANIUM POTASSIUM SILICATES $K_4M_2Si_6O_{18}$

LIN Z; FERREIRA A AND ROCHA J

J SOLID STATE CHEM

2003, 175, PP 258-263.

SYNTHESIS OF CONIFERINS ^{13}C -ENRICHED AT POSITIONS 4 AND 5 OF GUAIACYL RING

TERASHIMA N; EVTUGUIN D V; PASCOAL NETO C; PARKAS J

HOLZFORSCHUNG

2003, 57(5) PP 485-488

TETRABUTYLAMMONIUM 2,6-DIHYDROXYBENZOATE 2,6-DIHYDROXYBENZOIC ACID SOLVATE

ALMEIDA PAZ F A; SOARES-SANTOS P C R; NOGUEIRA H I S; TRINDADE T; KLINOWSKI J

ACTA CRYST

2003, E59, PP O506-O508.

THALLIUM π -CATION COMPLEXATION BY CALIX[4]TUBES: ^{205}Tl NMR AND X-RAY EVIDENCE

MATTHEWS S.E.; REES N. H.; V.FELIX; DREW M. G. B; BEER P. D.

INORGANIC CHEMISTRY

2003,42, PP. 729-734

THE EFFECT OF ACID MIXTURE ON THE STRUCTURE OF SOL-GEL PZT FIBERS, MEI ZHANG, I. M. MIRANDA SALVADO, PAULA M. VILARINHO MATERIALS LETTERS, (2003) 57, 26 & 27, 4271-4275

THE EFFECT OF COBALT OXIDE SINTERING AID ON ELECTRONIC TRANSPORT IN $CE_{0.80}GD_{0.20}O_{2-\delta}$ ELECTROLYTE

FAGG D P; ABRANTES J C C; PEREZ-COLL D; NUNEZ P; KHARTON V V; FRADE J R

ELECTROCHIM ACTA

2003, 48, PP 1023-1029

THE EFFECT OF TRIETHANOLAMINE ON THE FORMATION OF SOL-GEL DERIVED HYDROXYAPATITE/FLUOROAPATITE SOLID SOLUTION

CHENG K; WENG W; HAN G; DU P; SHEN G; YANG J AND FERREIRA J M F MATERIALS CHEMISTRY AND PHYSICS

2003, 78, PP 767-771.

THE FIRST ZINC(II) DITHIOCARBAMATO BIMETALLIC COMPLEX WITH BUTYL SUBSTITUENT GROUPS

ALMEIDA-PAZ F. A.; NEVES M. C.; TRINDADE T, KLINOWSKI J.

ACTA CRYST.

2003, E59, PP M1067-M1069.

THE FLUORAPATITE-ANORTHITE SYSTEM IN BIOMEDICINE

AGATHOPOULOS S; TULYAGANOV D U; MARQUES P A AP; FERRO MC;
FERNANDES M H V; CORREIA R N
BIOMATERIALS
2003, 24, PP 1317-1331

THE LP-MOCVD OF CDS/Bi₂S₃ BILAYERS USING SINGLE MOLECULE
PRECURSORS
MONTEIRO O. C.; TRINDADE T.; PARK J.H.; O'BRIEN P.
MATER. LETTERS
2003, 58, PP 119-122.

THE PRESSURE EFFECT ON THE WAX FORMATION ON DIESEL FUEL
PAULY, J., DARIDON, J.L., SANSOT, J.M., COUTINHO, J.A.P.
FUEL
2003, 82, PP 595-601.

THERMAL CONDUCTIVITY OF R365MFC MIXTURES
DOHRN R., HEINEMANN T., MARRUCHO I.M., OLIVEIRA N.
J. CELLULAR PLASTICS
2003, 39, PP 133 – 153

THERMAL AND CHEMICAL INDUCED EXPANSION OF LA_{0.3}SR_{0.7}(FE,GA)O_{3-δ}
CERAMICS
KHARTON V V; YAREMCHENKO A A; PATRAKEEV M V; NAUMOVICH E N;
MARQUES F M B
J EUROP CERAM SOC
2003, 23, PP 1417-1426

TRACER DIFFUSION COEFFICIENTS OF CITRAL AND D-LIMONENE IN
SUPERCRITICAL CARBON DIOXIDE.
FILHO C.A.; SILVA C.M.; QUADRI M.B.; MACEDO E.A.
FLUID PHASE EQUILIB.
2003, 204, PP 65-73

TRANSITION STATES FOR H ATOM TRANSFER REACTIONS IN THE
CH₂CH₂OH RADICAL: THE EFFECT OF A WATER MOLECULE
TEIXEIRA-DIAS, JJC; FURLANI, T R; SHORES, K S; GARVEY J F
PHYS CHEM CHEM PHYS
2003, 22 PP5063-5069.

TRAPPING CONTROL OF PHASE DEVELOPMENT IN ZONE MELTING OF
BSCCO SUPERCONDUCTING FIBRES
COSTA F M; CARRASCO M F; SILVA R F; VIEIRA J M
SUPERCOND SCI. TECHNOL
2003, 16, PP 392-397.

TRICRITICAL POINTS IN LA-BASED FERROMAGNETIC MANGANITES
AMARAL V. S., ARAÚJO J. P., POGORELOV YU. G., SOUSA J. B.,
TAVARES P. B., VIEIRA J. M., ALGARABEL P. A., IBARRA M. R.
JOURNAL OF APPLIED PHYSICS
2003, 93, PP 7646

TUNGSTOBORATES AS HIGHLY ACTIVE CATALYSTS FOR CYCLOALKANE OXYGENATION USING HYDROGEN PEROXIDE

SANTOS, I C M S; BALULA, M S; SIMÕES, M M Q; NEVES, M G P M S;
CAVALEIRO, J A S; CAVALEIRO, A M V
SYNLETT

2003, PP 1643-1646.

UNUSUAL ELECTROCHEMICAL REDUCTION OF COPPER (II) TO COPPER (I) FOR POLYOXOTUNGSTATE COMPOUNDS

GAMELAS, J. A F; BALULA, M S; CARAPUÇA, H M; CAVALEIRO, A M V
ELECTROCHEM COMMUN.

2003, 5, PP 378-382.

USE OF FTIR, FT-RAMAN AND ¹³C-NMR SPECTROSCOPIES FOR THE IDENTIFICATION OF SOME SEAWEED PHYCOCOLLOIDS

PEREIRA L; SOUSA A; COELHO H; AMADO A M; RIBEIRO-CLARO P J A
J. BIOMOL. ENGIN., 2003, 20, PP 223-228

USING PHASE DIAGRAMS TO DEAL WITH MOISTURE EXPANSION

SEGADÃES A M; CARVALHO M A; FERREIRA H C
CERAMICS INTERNATIONAL

2003, 29 [8] PP 947-954

VISCOSITY AND LIQUID DENSITY OF ASYMMETRIC HYDROCARBON MIXTURES

QUEIMADA, A.J., QUINÕES-CISNEROS, S.E., MARRUCHO, I.M. ,
COUTINHO, J. A. P. STENBY, E. H.,
INT J THERMOPHYS

2003, 21, PP 1221-1240.

WEAR RESISTANT CVD DIAMOND TOOLS FOR TURNING OF SINTERED HARDMETALS

BELMONTE M; FERRO P; FERNANDES A J S; COSTA F M; SACRAMENTO J;
SILVA R F

DIAMOND RELAT MATER

2003, 12, PP 738-743.

ARTIGOS NÃO SCI

ANÁLISE DA EXPANSÃO POR UMIDADE E ABSORÇÃO DE ÁGUA DE PISOS CERÂMICOS COMERCIAIS EM RELAÇÃO À COMPOSIÇÃO QUÍMICA E À QUANTIDADE DE FASE VÍTREA

MENEZES R R; FERREIRA H S; SEGADÃES A M; FERREIRA H C
CERÂMICA (SÃO PAULO)
2003, 49 [310] PP 72-81

ASPECTOS FUNDAMENTAIS DA EXTRUSÃO DE PASTAS CERÂMICAS VERMELHAS

RIBEIRO M J; FERREIRA A A; LABRINCHA J A
CERÂMICA INDUSTRIAL
2003, 8[1], PP 37-42.

CLAYS FROM SOUTHERN BRAZIL: PHYSICAL, CHEMICAL AND MINERALOGICAL CHARACTERIZATION

CORREIA S L; CURTO K A S; HOTZA D; SEGADÃES A M
PROCEEDINGS OF PTECH'03, GUARUJÁ-RJ, BRASIL
2003 (CD-ROM)

CONTEÚDOS DE ÁCIDO HEXENURÔNICO EM POLPAS KRAFT DE EUCALYPTUS GLOBULUS : VARIAÇÃO COM AS CONDIÇÕES DE POLPAÇÃO E EFEITO NA BRANQUEABILIDADE ECF

DANIEL A I D; PASCOAL NETO C; EVTUGUIN, D V ; SILVESTRE A J D
O PAPEL/TAPPI JOURNAL (ESPECIAL SUPL TECN.)
2003, nº 1 PP 4-12

CU-CE_{0.8}GD_{0.2}O_{2-D} MAERIALS AS SOFC ELECTROLYTE AND ANODE
FAGG D P, MATHER G C, FRADE J R
IONICS

2003, 9, PP 214-219

DESENVOLVIMENTO DE VIDRADOS PARA GRÉS PORCELÂNICO POLIDO
OLIVEIRA H J; SÃO MARCOS P; LABRINCHA J A
KERAMICA

2003, 258, MARÇO/ABRIL, PP 46-51.

DUAS DÉCADAS DE QUÍMICA INORGÂNICA EM AVEIRO. UMA VISÃO PESSOAL

CAVALEIRO, A M V
BOLETIM DA SOCIEDADE PORTUGUESA DE QUÍMICA
2003, 88, PP 31-36.

ELECTROCHEMICAL BEHAVIOR OF TI/AL₂O₃ INTERFACES PRODUCED BY DIFFUSION BONDING

ROCHA L A; ARIZA E; COSTA A M; OLIVEIRA F J AND SILVA R F
MATERIALS RESEARCH
2003, 6, 4, PP 439-444

GLASS AND SINTERED GLASS-CERAMICS FROM MUNICIPAL INCINERATOR WASTE

MONTEIRO, R. C. C., ALENDOURO, M. S., FIGUEIREDO, C. F., FERRO, M. C.,
FERNANDES, M. H. V,
WASCON 2003, ED. BY G. ORTIZ DE URBINA-INASMET AND H. GOUMANS-
ISCOWA,
2003, PP 553-559.

INCORPORATION OF CLAY-BASED CERAMIC FORMULATIONS
CONTAINING DIFFERENT SOLID WASTES
RIBEIRO M J; FERREIRA J M F AND LABRINCHA J A
EUROCERAM NEWS 14
([HTTP://WWW.EUROCERAM.ORG/EN/NEWS/NEWS_14_2.CFM](http://www.euROCERAM.org/en/news/news_14_2.cfm)), 2003, PP 1-4.

IR INVESTIGATION OF MULLITE SYNTHESIZED BY SOL-GEL
TECHNOLOGY, Y. DIMITRIEV, B. SAMUNOVA, I. M. SALVADO, E.
KASHCHIEVA, A. BACHVAROVA, J. OF THE UNIVERSITY OF CHEMICAL
TECHNOLOGY AND METALLURGY, XXXVIII, I (2003), PP 31-36

LA QUÍMICA EN LA EDUCACIÓN SECUNDARIA EN PORTUGAL: UNA
PERSPECTIVA DE CULTURA CIENTÍFICA
COSTA J A, MAGALHÃES M C, MARTINS I P, LOPES J M, SIMÕES M O,
SOBRINHO T
ALAMBIQUE, DIDÁCTICA DE LAS CIENCIAS EXPERIMENTALES
2003, 36, PP 68-75

MIXED CONDUCTIVITY OF GADOLINIUM TITANATE-BASED
PYROCHLORE CERAMICS: THE GRAIN BOUNDARY EFFECTS
KHARTON V V; MARQUES F M B; TSIPIS E V; VISKUP A P; PATRAKEEV M
V; HARKAVY A V; SAMIGULLINA R; FRADE J R
IONICS
2003, 9, PP 122-126

MIXED CONDUCTIVITY OF ZIRCON-TYPE $CE_{1-x}A_xVO_{4\pm\delta}$ (A = CA, SR)
TSIPIS E V; KHARTON V V; VYSHATKO N P; SHAULA A L; PATRAKEEV M
V; FRADE J R
IONICS
2003, 9, PP 231-237

MOISTURE EXPANSION: ACTIVATION ENERGY VERSUS FIRING
TEMPERATURE
CARVALHO M A; SEGADÃES A M
PROCEEDINGS OF ECERS'03, ISTANBUL, TURQUIA
2003, EUROPEAN CERAMIC SOCIETY

OS POLIOXOMETALATOS. DO ANIÃO DE KEGGIN ÀS NANOCÁPSULAS
GAMELAS, J; CAVALEIRO, A; SANTOS, I; BALULA, M S
BOLETIM DA SOCIEDADE PORTUGUESA DE QUÍMICA
2003, 90, PP 45-51

PREPARATION OF NANOSIZED LA1-XSRXMNO3 POWDERS
A. STANEVA, J.M. VIEIRA, Y. IVANOVA, M. KOSTOVA, L. YAND, E. GATTEF
, Y. DIMITRIEV

NANOSCIENCE AND NANOTECHNOLOGY 3,
EDS. E. BALABANOVA AND I. DRAGIEVA
HERON PRESS, SOFIA,
2003, PP 70-72

QUESTIONS OF CHEMISTRY
PEDROSA DE JESUS, H; TEIXEIRA-DIAS, J J C; WATTS, M
INT J SCI EDUC
2003, 25 PP1015-1034

QUÍMICA DE MATERIAIS LENHOCELULOSICOS NA UNIVERSIDADE DE
AVEIRO: BREVE REVISÃO DE UMA DÉCADA DE INVESTIGAÇÃO
PASCOAL NETO C ; EVTUGUIN D V.
BULL. SPQ
2003, 88 PP37-46

RECYCLING OF GRANITE SLUDGES IN BRICK-TYPE AND FLOOR TILE-
TYPE CERAMIC FORMULATIONS
FERREIRA J M F; TORRES P M C; SILVA M S AND LABRINCHA J A
EUROCERAM NEWS 14
([HTTP://WWW.EUROCERAM.ORG/EN/NEWS/NEWS_14_1.CFM](http://www.euroceram.org/en/news/news_14_1.cfm)), 2003, PP 1-5.

REFRACTORY FORMULATIONS MADE OF DIFFERENT WASTES AND
NATURAL SUB-PRODUCTS
PEREIRA F R; NUNES A F; SEGADÃES A M; LABRINCHA J A
PROCEEDINGS OF ECERS'03, ISTANBUL, TURQUIA
2003, EUROPEAN CERAMIC SOCIETY

REUTILIZAÇÃO *IN SITU* DAS LAMAS RESIDUAIS DE UMA INDÚSTRIA
CERÂMICA
COSTA M G; RIBEIRO M J P; LABRINCHA J A
KERAMICA
2003, 259, MAIO/JUNHO, PP 34-42.

REUTILIZACIÓN DE GRANALLA DE DESBASTE DE LA INDUSTRIA NAVAL
EN LA FABRICACIÓN DE CEMENTO PORTLAND
RIBEIRO M J P; GULÍAS M R; LABRINCHA J A
RESIDUOS
2003, 74[9-10], PP 96-98.

SINGLE-SOURCE METHODS FOR THE PREPARATION OF
NANOCRYSTALLINE SEMICONDUCTORS
TRINDADE T.
COLOIDES E INTERFACES, EDS. LIZ-MARZÁN L. M.; HERVÉS P.; MEJUTO J.
C.; TOJO C.; UNIVERSIDADE DE VIGO, 2003, 147.

SOLUBILIDAD DE GASES EN PERFLUOROALCANOS LINEALES:
PREDICCIONES DE LA ECUACIÓN DE ESTADO SOFT-SOFT
DIAS, A.M.A., PÀMIES, J.C., COUTINHO, J.A.P., MARRUCHO, I.M., VEGA, L.F.

PROCEEDINGS OF THE III JORNADAS NACIONALES DE INGENIERÍA
TERMODINÁMICA. VALÈNCIA, ESPANHA, JUNHO 2003.
2003, ED UPV.

USING EXPERIMENTS DESIGN TO MODEL LINEAR FIRING SHRINKAGE OF
TRIAxIAL CERAMIC BODIES
CORREIA S L; CURTO K A S; HOTZA D; SEGADÃES A M
PROCEEDINGS OF PTECH'03, GUARUJÁ-RJ, BRASIL
2003 (CD-ROM)

CAPÍTULOS DE LIVROS DE EDITORA INTERNACIONAL

APPLICATION OF NMR AND HYPHENATED NMR SPECTROSCOPY FOR THE
STUDY OF BEER COMPONENTS
DUARTE IF ; SPRAUL M ; GODEJOHANN M AND GIL AM
MAGNETIC RESONANCE IN FOOD SCIENCE - LATEST DEVELOPMENTS
EDS. WEBB, G.A., BELTON, P.S., GIL, A.M., RUTLEDGE, D.N.,
THE ROYAL SOCIETY OF CHEMISTRY, CAMBRIDGE,
2003; PP 151-157. ISBN 0-85404-886-3.

CHEMICAL ASPECTS OF SEMICONDUCTOR NANOCRYSTALS
TRINDADE T.
EDS. LIZ-MARZÁN L. M.; KAMAT P. V.
KLUWER ACADEMIC PUBLISHERS
2003, CHP , P.P. 157-179.

HANDBOOK OF ORGANIC-INORGANIC HYBRID MATERIALS AND
NANOCOMPOSITES
CARLOS L D, BERMUDEZ DE ZEA V, SÁ FERREIRA R A
EDS. NALWA, H. S.
AMERICAN SCIENTIFIC PUBLISHERS, LA, USA
2003, VOL 1, CHP 9, PP 353-380.

SPECTROSCOPY: NUCLEAR MAGNETIC RESONANCE
GIL, A.M.
ENCYCLOPEDIA OF FOOD SCIENCES AND NUTRITION,
2003, 2ND EDITION, ACADEMIC PRESS, PP 5447-545

TECHNIQUES FOR ANALYSING WHEAT PROTEINS
GIL AM
BREAD MAKING – IMPROVING QUALITY

ED. CAUVAIN, S.P.
WOODHEAD PUBLISHING LIMITED AND CRC PRESS
2003; CHP 5, PP 97-120. ISBN 0-8493-1762-2.

CAPÍTULOS DE LIVROS DE EDITORA NACIONAL

BIOMATERIAIS CERÂMICOS
CORREIA R N
IN MATERIAIS 2000,
EDS. FORTES M A; FERREIRA P
IST PRESS
2003, PP 401-410

CERÂMICOS ESTRUTURAIIS
J.M. VIEIRA
IN “MATERIAIS DOIS MIL”,
EDS. M. AMARAL FORTES, P.J. FERREIRA,
IST PRESS, LISBON
2003, CAP 2.1, PP 79-87

COMPÓSITOS DE MATRIZ CERÂMICA
SILVA R F
“MATERIAIS 2000”, CAP. 4.2.
EDS. FERREIRA P J; AMARAL FORTES E M
IST PRESS
2003, PP 191-200.

CONDUTORES IÓNICOS
FIGUEIREDO F.M., MARQUES F.M.B., FRADE J.R.
IN MATERIAIS 2000
EDS. M.A. FORTES, P.J. FERREIRA, IST PRESS
2003, PP. 353-361.

MATERIAIS COM MAGNETORESISTÊNCIA COLOSSAL
AMARAL, V. S.
IN “OS MATERIAIS DOIS MIL” ,
EDS. AMARAL FORTES, M. ; FERREIRA, P. J.
IST PRESS
2003, CAP 5.2, PP 249-257

MATERIAIS FERROELÉCTRICOS

P. M. VILARINHO, E. JOANNI

OS MATERIAIS NOS ANOS 2000, CAPÍTULO 6, PAG. 329 – 338,
EDITADO POR M. AMARAL FORTES, P. J. PEREIRA,
IST PRESS, LISBOA, 2003.

MATERIAIS PIEZOELECTRICOS

KHOLKIN A L; BAPTISTA J L

EM MATERIAIS 2000, EDS. FONTES M. A; FERREIRA P. J.,
IST PRESS, LISBOA, 550 P, ISBN: 972-8469-23-3
2003, CHP 6.6

SENSORES DE OXIGÉNIO F.M.B. MARQUES, J.R. FRADE, J.A.
LABRINCHA, IN MATERIAIS DOIS MIL E UM,
ED. A. FORTES, P. FERREIRA, LISBOA
INSTITUTO SUPERIOR TÉCNICO, (2003).

SENSORES QUÍMICOS

MARQUES F.M.B., LABRINCHA J.A, FRADE J.R.
IN MATERIAIS 2000
EDS. M.A. FORTES, P.J. FERREIRA, IST PRESS,
2003, PP. 491-498.

PATENTES NACIONAIS

ELÉCTRODO TIPO SECO PARA MONITORIZAÇÃO DE BIO-POTENCIAIS,
BARBOSA, M, MARQUES DE SÁ J, FONSECA J C, FERREIRA V M, SALVADO
I M, MARTINS R M, CUNHA J M, SILVA A M,
PATENTE CONJUNTA ENTRE UNIVERSIDADE DE AVEIRO, INEB-PORTO E
O HOSPITAL DE STO ANTÓNIO-PORTO,
PORTUGAL, PATENT N° 102999, JULHO 2003.

MÉTODO DE PRODUÇÃO DE FILMES ESPESSOS COMPÓSITOS CERÂMICOS
POR
SEDIMENTAÇÃO E INFILTRAÇÃO DE SOLUÇÕES SOL-GEL"
VILARINHO P M; WU A; KHOLKIN A
REGISTO DE PATENTE DE INVENÇÃO NACIONAL, N.º 102 909, 13 DE
FEVEREIRO DE 2003.

TAPE CASTING EM MEIO AQUOSO DE SUBSTRATOS VITRO-CERÂMICOS À
BASE DE CORDIERITE COM BAIXA CONSTANTE DIELECTRICA
FERREIRA J M F; MEI S
PATENTE PORTUGUESA, N.º. 103 021.

PROCEEDINGS DE CONF. INTERNACIONAL (≥ 4 PÁGINAS)

A COMPARISON OF ACTIVITY COEFFICIENT MODELS FOR CORRELATION OF SOLVENT ACTIVITIES IN POLYMER SOLUTIONS

PEDROSA, N., GAO, J., MARRUCHO, I.M., COUTINHO, J.A.P.,
PROCEEDINGS OF THE 20TH EUROPEAN SYMPOSIUM ON APPLIED THERMODYNAMICS, LAHNSTEIN, ALEMANHA, OUTUBRO 2003.
2003, VDI, PP 407-410

A CORRESPONDING STATES MODEL FOR THE ESTIMATION OF THERMOPHYSICAL PROPERTIES OF ASYMMETRIC MIXTURES.

QUEIMADA, A.J., MARRUCHO, I.M., STENBY, E.H., COUTINHO, J.A.P.,
PROCEEDINGS OF THE 20TH EUROPEAN SYMPOSIUM ON APPLIED THERMODYNAMICS, LAHNSTEIN, ALEMANHA, OUTUBRO 2003.
2003, VDI, PP 383-386

A MODIFIED EXTENDED UNIQUAC MODEL FOR PROTEINS

COUTINHO, J.A.P., PESSOA, F.L.P., 2003..
PROCEEDINGS OF THE 15TH SYMPOSIUM ON THERMOPHYSICAL PROPERTIES. BOULDER, EUA, JUNHO 2003.
2003, NIST.

AN IMPROVED ¹³C TRACER METHOD FOR THE STUDY OF LIGNIN STRUCTURE AND REACTIONS

TERASHIMA N; EVTUGUIN D V; PASCOAL NETO C; PARKAS J; PAULSSON M; WESTERMARK U; RALPH S; RALPH J
PROCEEDINGS OF 12TH ISWPC, MADISON, USA,
2003, VOL 1, Pp 175-178

ANALYSIS OF THE CREEP BEHAVIOUR OF POLYPROPYLENE

ANDRÉ J R S AND CRUZ PINTO J J C
APHYS – 2003 INTERNATIONAL CONFERENCE, 12-18 OCTOBER 2003,
BADAJOZ, SPAIN, 6 PP

APPLICATION OF FTIR SPECTROSCOPY FOR THE QUANTIFICATION OF SUGARS IN MANGO JUICE AS A FUNCTION OF RIPENING

DUARTE, I.F., BARROS, A., DELGADILLO, I. AND GIL, A.M.
6º ENCONTRO DE QUÍMICA DE ALIMENTOS, JUNHO 2003, LISBOA.
VOLUME I, PP 454-458.

ATMOSPHERIC GASES AND AROMAS IN BIODEGRADABLE PACKAGING
OLIVEIRA, N. S., FERREIRA, A., LOPES DA SILVA, J. A., MARRUCHO, I. M.

PROCEEDINGS OF THE 20TH ESAT: EUROPEAN SYMPOSIUM ON APPLIED THERMODYNAMICS. LAHNSTEIN, ALEMANHA, OUTUBRO 2003. 2003, VDI, PP 183-186

CERAMICS AND GLASSES IN MEDICINE: A CHEMICAL AND STRUCTURAL APPROACH

AGATHOPOULOS S; TULYAGANOV D AND FERREIRA J M F
AL-AZHAR BULLETIN OF SCIENCE, PROCEEDINGS OF 5TH INT. SCI. CONF., 25-27 MARCH
2003, PP 103-114.

CREEP BEHAVIOUR OF VISCOELASTIC POLYMER MATERIALS

ANDRÉ J R S AND CRUZ PINTO J J C
MATERIAIS 2003
II INTERNATIONAL MATERIALS SYMPOSIUM, 14-16 APRIL 2003, FCT-UNL, CAPARICA, PORTUGAL
4 PP

DENSIFICATION OF SIO₂-ZRO₂ XEROGELS BT ADDITION OF FRESH SOLS BEFORE GELATION, I.M.MIRANDA SALVADO, J. SANTOS SOUSA, F.M.A. MARGAÇA, J. TEIXEIRA;
PROCEEDINGS DO 47º CONGRESSO BRASILEIRO DE CERÂMICA, JOÃO PESSOA, BRASIL,
15-18 JUNHO 2003 PP 2026-2035

ECF BLEACHING RESPONSE OF E. GLOBULUS KRAFT PULPS: INFLUENCE OF PULPING CONDITIONS AND RELATIONSHIP WITH CHEMICAL STRUCTURE OF PULPS

PASCOAL NETO C; EVTUGUIN D V; DANIEL A I D; SILVESTRE A;
FURTADO F P; MENDES SOUSA P
PROCEEDINGS OF 28TH EUCEPA SYMP, LISBON, PORTUGAL,
2003, PP 35-40

ENZYMATIC METHOD FOR DETERMINING OXYGEN SOLUBILITY IN PERFLUOROCARBON EMULSIONS

FREIRE, M.G., DIAS, A.M.A., COUTINHO, J.A.P., COELHO, M.A.Z., MARRUCHO, I.M.,
PROCEEDINGS OF THE 20TH EUROPEAN SYMPOSIUM ON APPLIED THERMODYNAMICS, LAHNSTEIN, ALEMANHA, OUTUBRO 2003.
2003, VDI, PP 215-218

GAS POLYMER SOLUBILITY USING A QUARTZ CRYSTAL MICROBALANCE.

OLIVEIRA, N.S., JUN, G., BARROS, A., COUTINHO, J.A.P., DARIDON, J.L., MARRUCHO, I.M.,
PROCEEDINGS OF THE 20TH EUROPEAN SYMPOSIUM ON APPLIED THERMODYNAMICS, LAHNSTEIN, ALEMANHA, OUTUBRO 2003.
2003, VDI, PP 11-14

GENERALIZED RELATION BETWEEN SURFACE TENSION AND VISCOSITY:
A STUDY ON PURE AND MIXED N-ALKANES
QUEIMADA, A.J., MARRUCHO, I.M., STENBY E.H., COUTINHO, J.A.P., 2003..
PROCEEDINGS OF THE 15TH SYMPOSIUM ON THERMOPHYSICAL
PROPERTIES. BOULDER, EUA, JUNHO 2003.
2003, NIST.

IMPROVING THE COMPATIBILITY OF PINE, EUCALYPT AND CORK WITH
PORTLAND CEMENT FOR THE MANUFACTURE OF PANEL PRODUCTS
PEREIRA C; JORGE F C; IRLE M AND FERREIRA J M F
PROCEEDINGS OF THE SEVENTH PANEL PRODUCTS SYMPOSIUM,
LLANDUDNO, WALES, UK, 8-10 OCTOBER 2003, ED. BY BIOCOMPOSITE
CENTRE, UWB, BANGOR, ISBN: 184 220 057 7
2003, PP 26-37.

INFLUENCE OF PARAMETERS CONNECTED WITH MIXING AND
APPLICATION PROCESSES OF ONE-COAT RENDER, WITH AIR-
ENTRAINING AGENTS, ON THE PROPERTIES OF FRESH MORTAR AND
HARDENED MORTAR
SILVA L, FERNANDES V, FERREIRA V M
PROCEEDINGS OF THE 2ND INTERNATIONAL SYMPOSIUM ON BUILDING
PATHOLOGY, DURABILITY AND REHABILITATION, LISBON, PORTUGAL,
EDIÇÕES LNEC,
2003, theme 4, PP 547-556.

INFLUENCE OF WOOD PULPING CONDITIONS AND UNBLEACHED PULP
COMPOSITION AND STRUCTURE ON THE *ecf* BLEACHABILITY OF
HARDWOOD KRAFT PULPS
PASCOAL NETO C ; EVTUGUIN D V; DANIEL A I D; SILVESTRE A J D;
FURTADO F P; MENDES SOUSA P
PROCEEDINGS OF INTERNATIONAL COLLOQUIUM ON EUCALYPTUS
KRAFT PULP, VIÇOSA, BRASIL
2003, PP 163-179

KRAFT PULPING BEHAVIOUR OF XYLANS FROM *EUCALYPTUS GLOBULUS*,
EUCALYPTUS UROGRANDIS AND *BETULA VERRUCOSA* DURING
PINTO P; EVTUGUIN D V; PASCOAL NETO C
PROCEEDINGS OF 12TH ISWPC, MADISON, USA
2003, VOL. 2, PP 87-90

LOCAL ELECTROMECHANICAL PROPERTIES AND GRAIN SIZE EFFECTS IN
FERROELECTRIC RELAXORS STUDIED BY SCANNING PIEZOELECTRIC
MICROSCOPY
KHOLKIN A. L; SHVARTSMAN V. V.; WOITAS M.; SAFARI A.
MATERIALS.
RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS

MECHANICAL BEHAVIOUR OF ROLLED AA1050 UNDER UNIAXIAL
TENSION AT DIFFERENT TEMPERATURES
MALIK H, ALI N, LOPES AB, BARLAT F AND GRACIO JJ

PROCEEDINGS FOR THE 8TH INTERNATIONAL SYMPOSIUM ON
ADVANCED MATERIALS, ISLAMABAD, PAKISTAN, 2003.

MODELLING OF THE WATER-HYDROCARBON INTERFACIAL TENSION:
COUPLING THE CPA EOS WITH THE GRADIENT THEORY.
QUEIMADA, A.J., MARRUCHO, I.M., STENBY, E.H., KONTOGEOGRIS, G.M.,
MIQUEU, C., COUTINHO, J.A.P.,
PROCEEDINGS OF THE 20TH EUROPEAN SYMPOSIUM ON APPLIED
THERMODYNAMICS, LAHNSTEIN, ALEMANHA, OUTUBRO 2003.
2003, VDI, PP 391-394

MULTIVARIATE ANALYSIS OF FTIR AND NMR DATA OF BEER AS A
POTENTIAL TOOL FOR ITS QUALITY CONTROL ALMEIDA, C., DUARTE,
I.F., BARROS, A. AND GIL, A.M.
6^º ENCONTRO DE QUÍMICA DE ALIMENTOS, JUNHO 2003, LISBOA.
VOLUME I, PP 424-427.

NANOSCALE CHARACTERIZATION AND LOCAL ELECTROMECHANICAL
PROPERTIES OF FERROELECTRIC FILMS FOR MEMS
KHOLKIN A. L.; SHVARTSMAN V. V.; EMELYANOV A. YU., SAFARI A.
PROCEEDINGS OF THE ELECTROCHEM. SOCIETY MEETING, SYMPOSIUM
“DIELECTRICS IN EMERGING TECHNOLOGIES”, PARIS, FRANCE, APR. 27-
MAY 2, 2003, PP. 145-160.

NEW COMPLEMENTARY INFORMATION ON THE *E. GLOBULUS* LIGNIN
STRUCTURE OBTAINED BY ¹³C SELECTIVE LABELLING AND ADVANCED
NMR TECHNIQUES
EVTUGUIN D V; BALAKSHIN M YU; TERASHIMA N; PASCOAL NETO C ;
SILVA A S M
PROCEEDINGS OF 12TH ISWPC, MADISON, USA
2003, VOL 3, PP177-180

OXYGEN TRANSPORT AND ELECTROCHEMICAL ACTIVITY OF LA₂NIO₄-
BASED CATHODE MATERIALS
KHARTON V V; YAREMCHENKO A A; TSIPI S E V; FRADE J R
PROCEEDINGS OF INTERNATIONAL SYMPOSIUM “SOFC-VIII”, PARIS, EDS:
SINGHAL S C; DOKIYA M
2003, THE ELECTROCHEMICAL SOCIETY, PENNINGTON, PROCEEDINGS
VOLUME 2003-07, PP 561-570

PERFLUOROCARBONS AS AN AGENT FOR IMPROVE PRODUCTIVITY IN
YEAST CULTIVATION
COELHO, M.A.Z., AMARAL, P.F.F., TAVARES, A.P.M., FREIRE, MARRUCHO,
I.M., COUTINHO, J.A.P.,
PROCEEDINGS OF THE 20TH EUROPEAN SYMPOSIUM ON APPLIED
THERMODYNAMICS, LAHNSTEIN, ALEMANHA, OUTUBRO 2003.
2003, VDI, PP 233-236

PULP BLEACHING CATALYSED BY POLYOXOMETALATES – PAST,
PRESENT AND FUTURE
EVTUGUIN D V; GASPAR A ; PASCOAL NETO C

PROCEEDINGS OF 28TH EUCEPA SYMP, LISBON, PORTUGAL
2003, PP 74-78

RECENT ADVANCES IN THE MICROSCOPIC CHARACTERIZATION OF
MATERIALS

MATOS M. J.; VILARINHO P. M.; KHOLKIN A. L.

ACTAS DO 3º CONGRESSO LUSO-MOÇAMBICANO DE ENGENHARIA,
MAPUTO, MOÇAMBIQUE,
2003, PP 587 – 594

RECYCLING OF INDUSTRIAL RESIDUES - THE BEST STRATEGY FOR
WASTE MANAGEMENT

FERREIRA J M F; GUEDES P J S AND FAIM P F

AL-AZHAR BULLETIN OF SCIENCE, PROCEEDINGS OF 5TH INT. SCI. CONF.,
25-27 MARCH
2003, PP 293-305.

RECYCLING OF SEVERAL WASTES AS REFRACTORY MATERIALS

PEREIRA F R; HOTZA D; SEGADÃES A M; LABRINCHA J A

PROCEEDINGS OF UNITECR'03 (8TH BIENNIAL WORLDWIDE CONGRESS ON
REFRATORIES), OSAKA, JAPÃO
2003, TARJ, PP 150-153.

RELAÇÕES ENTRE DISTRIBUIÇÃO GRANULOMÉTRICA, MORFOLOGIA E
EMPACOTAMENTO DE PARTÍCULAS NUM SISTEMA REAL: ALTA-
ALUMINA

SILVA A P; SEGADÃES A M; DEVEZAS T C

ACTAS DO 47º CONGRESSO BRASILEIRO DE CERÂMICA, JOÃO PESSOA-PB,
BRASIL
2003, ASSOCIAÇÃO BRASILEIRA DE CERÂMICA (CD-ROM, 1-16), PP 150-
161.

RELATIONSHIPS BETWEEN COATING CHARACTERISTICS AND
PRINTABILITY

CONCEIÇÃO S I; SANTOS N; VELHO J L; KHOLKIN A AND FERREIRA J M F

PROCEEDINGS OF THE INTERNATIONAL CONFERENCE WPP 2003 ON
CHEMICAL TECHNOLOGY OF WOOD, PULP AND PAPER, BRATISLAVA,
SETEMBER 17-19, SLAVAKIA
2003, PP.161-166.

RESÍDUOS INDUSTRIAIS COMO ALTERNATIVA A RECURSOS MINERAIS

PEREIRA F R; LABRINCHA J A; SEGADÃES A M; HOTZA D; ACCHAR W

ACTAS DO 47º CONGRESSO BRASILEIRO DE CERÂMICA, JOÃO PESSOA-PB,
BRASIL
2003, ASSOCIAÇÃO BRASILEIRA DE CERÂMICA (CD-ROM, 19-20), PP 2398-
2410.

ROLE OF GRAIN BOUNDARIES IN OXYGEN IONIC TRANSPORT IN MIXED-CONDUCTING CERAMICS

KHARTON V V; YAREMCHENKO A A; VISKUP A P; FIGUEIREDO F M; KOVALEVSKY A V; NAUMOVICH E N; MARQUES F M B

GRAIN BOUNDARY ENGINEERING OF ELECTRONIC CERAMICS

PROCEEDINGS OF COST 525 MEETING, AVEIRO, EDS: FREER R; VAN HERLE J; PETZELT J; LEACH C

2003, MANEY LEEDS, UK, BRITISH CERAMIC PROCEEDINGS, NO 63, PP 27-36

SELF-ORGANIZATION PHENOMENA IN PULSED LASER ANNEALED SI/GE SUPERLATTICES

SOBOLEV N. A., IVLEV G. D., GATSKEVICH E. I., SHARAEV D. N., LEITÃO J. P., FONSECA A., CARMO M. C., LOPES A. B., SHVARTSMAN V. V., KHOLKIN A. L., KIBBEL H., PRESTING H.

PROCEEDINGS OF NANOMEETING'2003, ED. BORISENKO V. E.,

GAPONENKO S. V., GURIN V. S. MINSK, BELARUS, MAY 20-23, 2003, PP. 496-499.

SINTERIZAÇÃO RÁPIDA DO Al_2TiO_5 OBTIDO POR COMBUSTÃO

FERREIRA H S; SEGADÃES A M; KIMINAMI R H G A

ACTAS DO 47º CONGRESSO BRASILEIRO DE CERÂMICA, JOÃO PESSOA-PB, BRASIL

ASSOCIAÇÃO BRASILEIRA DE CERÂMICA (CD-ROM, 9-20)

2003, PP 1581-1592.

SOLUBILIDAD DE GASES EN PERFLUOROALCANOS LINEALES:

PREDICIONES DE LA ECUACIÓN DE ESTADO SOFT-SOFT

DIAS, A.M.A., PÀMIÉS, J.C., COUTINHO, J.A.P., MARRUCHO, I.M., VEGA, L.F.

PROCEEDINGS OF THE III JORNADAS NACIONALES DE INGENIERÍA

TERMODINÁMICA. VALÈNCIA, ESPANHA, JUNHO 2003.

2003, ED UPV.

SOLUBILITY OF GASES IN PERFLUOROALKANES: EXPERIMENTS AND MODELLING

DIAS, A.M.A., COUTINHO, J.A.P., MARRUCHO, I.M., PÀMIÉS, J.C., VEGA, L.F.,

PROCEEDINGS OF THE 20TH EUROPEAN SYMPOSIUM ON APPLIED

THERMODYNAMICS, LAHNSTEIN, ALEMANHA, OUTUBRO 2003.

2003, VDI, PP 199-202

SOLUBILITY OF OXYGEN IN LIQUID PERFLUOROCARBONS.

DIAS, A.M.A., FREIRE, M., COUTINHO, J.A.P., MARRUCHO, I.M.,

2003 PROCEEDINGS OF THE 15TH SYMPOSIUM ON THERMOPHYSICAL PROPERTIES. BOULDER, EUA, JUNHO 2003.

2003, NIST.

STRUCTURAL AND ELECTRICAL CHARACTERIZATION OF PZT SEEDED FILMS

WU A., VILARINHO P. M., SALVADO I. M., KHOLKIN A. L., BAPTISTA J. L.

BRITISH CERAMIC PROCEEDINGS NO. 63: GRAIN BOUNDARY
ENGINEERING OF ELECTRONIC CERAMICS, ED. R. FREER, J. VAN HERLE,
J. PETZELT, AND C. LEACH,
2003, PP 155-162

STRUCTURAL TRANSFORMATIONS OF LIPOPHILIC EXTRACTIVES
DURING EUCALYPTUS GLOBULUS KRAFT PULP BLEACHING
FREIRE C S R; SILVESTRE A J D AND NETO C P
PROCEEDINGS BOOK OF THE 12TH INT SYMP WOOD PULPING CHEM,
MADISON, USA
2003, VOL I, PP 125-128

STRUCTURE OF NANODOMAINS IN RELAXORS
VAKHRUSHEV S. B., NABEREZHNOV A. A., DKHIL B., KIAT J.-M.,
SHVARTSMAN V., KHOLKIN A., DORNER B., IVANOV A.
AIP PROCEEDINGS.
2003, 677, P 74

STUDY ON LIGNIN REACTIONS IN OXYGEN DELIGNIFICATION
CATALYSED BY Mn(II) ASSISTED POLYOXOMETALATES
GASPAR A; EVTUGUIN D V; PASCOAL NETO C
PROCEEDINGS OF 12TH ISWPC, MADISON, USA
2003, VOL. 2, PP 83-86

STUDY OF PERFLUOROCARBON EMULSIONS STABILITY USING IMAGE
ANALYSIS
FREIRE, M.G., DIAS, A., COELHO, M.A.Z., COUTINHO, J.A.P., MARRUCHO,
I.M.
PROCEEDINGS OF THE 20TH EUROPEAN SYMPOSIUM ON APPLIED
THERMODYNAMICS, LAHNSTEIN, ALEMANHA, OUTUBRO 2003.
2003, VDI, PP 211-214

STUDY OF THE STABILITY AND OXYGEN SOLUBILITY OF
PERFLUOROCARBON EMULSIONS
FREIRE, M., DIAS, A.M.A., FREIRE, M., COELHO, M.A.Z., COUTINHO, J.A.P.,
MARRUCHO, I.M., 2003.
PROCEEDINGS OF THE 15TH SYMPOSIUM ON THERMOPHYSICAL
PROPERTIES. BOULDER, EUA, JUNHO 2003.
2003, NIST.

THE INFLUENCE OF REOLOGY ON PAPER COATING PROPERTIES CONCEIÇÃO S I;
SANTOS N; VELHO J L AND FERREIRA J M F
PROCEEDINGS FO THE INTERNATIONAL CONFERENCE WPP 2003 ON CHEMICAL
TECHNOLOGY OF WOOD, PULP AND PAPER, BRATISLAVA, SETEMBER 17-19, SLAVAKIA
2003, PP 199-204.

THE PHASE DIAGRAM OF THE TERNARY FLUORAPATITE-ANORTHITE-
DIOPSIDE SYSTEM AND ITS APPLICATION FOR PRODUCING GLASSES
AND GLASS-CERAMICS
TULYAGANOV D; AGATHOPOULOS S AND FERREIRA J M F
AL-AZHAR BULLETIN OF SCIENCE, PROCEEDINGS OF 5TH INT. SCI. CONF.,
25-27 MARCH

2003, PP 115-126.

THERMODYNAMIC PROPERTIES OF PERFLUOROCARBONS.

DIAS, A.M.A., COUTINHO, J.A.P., MARRUCHO, I.M., SANTOS, L.B., PIÑEIRO, M.

PROCEEDINGS OF THE 15TH SYMPOSIUM ON THERMOPHYSICAL PROPERTIES. BOULDER, EUA, JUNHO 2003
2003, NIST.

TOWARDS BETTER UNDERSTANDING OF LIGNIN ASSEMBLY: THE ASSESSMENT OF THE SEQUENTIAL ORDER OF BUILDING BLOCKS AND INTERUNIT LINKAGES USING ELECTROSPRAY IONIZATION MASS SPECTROMETRY.

EVTUGUIN D V AND AMADO F M L

PROCEEDINGS OF 12TH ISWPC, MADISON, USA,
2003, VOL 1, PP 277-280

UTILIZATION OF SOLID WASTES FROM GRANITE CUTTING PROCESSING IN PORCELAIN INDUSTRY

FERNANDES H R; TORRES P; AGATHOPOULOS S; TULYAGANOV D AND FERREIRA J M F

AL-AZHAR BULLETIN OF SCIENCE, PROCEEDINGS OF 5TH INT. SCI. CONF., 25-27 MARCH
2003, PP 33-43.

VISCOSITY AND LIQUID DENSITY OF ASYMMETRIC N-ALKANE MIXTURES: MEASUREMENT AND MODELLING

QUEIMADA, A.J., MARRUCHO, I.M., COUTINHO, J.A.P., STENBY, E.H., 2003..

PROCEEDINGS OF THE 15TH SYMPOSIUM ON THERMOPHYSICAL PROPERTIES. BOULDER, EUA, JUNHO 2003.
2003, NIST.

PROCEEDINGS DE CONFERÊNCIA NACIONAL OU INTERNACIONAL INFERIOR A 4 PÁGINAS

A COMPARATIVE STUDY OF IONIC AND ELECTRONIC TRANSPORT IN AL-W(MO)-O PHASES

SMIRNOVA O A; MAROZAU I P; VISKUP A P; KHARTON V V;

NAUMOVICH E N; MARQUES F M B

ABSTRACTS OF THE OSSEP WORKSHOP "IONIC AND MIXED CONDUCTORS: METHODS AND PROCESSES"

2003, AVEIRO, P 14

A LUMINESCÊNCIA DO IÃO Eu^{3+} COMO SONDA ESTRUTURAL

CARLOS L D

ORAL COMMUNICATION: 3º ENCONTRO NACIONAL DE TERRAS RARAS, INSTITUTO DE QUÍMICA, UNESP, ARARAQUARA, S.P., BRASIL (2003)

A MINA DE OURO DE SANTO ANTÓNIO – PENEDONO. CONSEQUÊNCIAS AMBIENTAIS DA EXPLORAÇÃO MINEIRA E SEU ABANDONO
MATIAS M J, ABREU M M, SANTOS OLIVEIRA J M, MAGALHÃES M C, BASTO M J, ÁVILA P, JOAQUIM C
IV CONGRESSO IBÉRICO DE GEOQUÍMICA E XIII SEMANA DE GEOQUÍMICA,
UNIVERSIDADE DE COIMBRA, DEPARTAMENTO DE CIÊNCIAS DA TERRA, COIMBRA 14 A 18 DE JULHO DE 2003
LIVRO DE RESUMOS, PP 337-339

A RAMAN AND SOLID-STATE NMR SPECTROSCOPIC STUDY OF CRYSTALLINE AND GLASSY GLUCOSE, ANA M. AMADO, ANDREIA ROSA, L. HILLIOU, ANA M. GIL AND PAULO J.A. RIBEIRO-CLARO, 5º ENCONTRO INTERNACIONAL DO GRUPO DOS GLÚCIDOS DA SPQ, 7-10 SETEMBRO 2003, COVILHÃ. P 25 (1 PÁGINA)

A SOLID STATE NMR AND RAMAN SPECTROSCOPY STUDY OF CRYSTALLINE AND GLASSY GLUCOSE, A. ROSA, L. HILLIOU, A.M.AMADO, P.J.A.RIBEIRO-CLARO AND A.M.GIL, THE 3RD ALPINE CONFERENCE ON SOLID-STATE NMR, SETEMBRO 14-18 2003, CHAMONIX-MONT BLANC, FRANCE (1 PÁGINA).

A SOLID STATE NMR AND RAMAN SPECTROSCOPY STUDY OF CRYSTALLINE AND GLASSY GLUCOSE, A. ROSA, L. HILLIOU, A.M.AMADO, P.J.A.RIBEIRO-CLARO AND A.M.GIL, II ENCONTRO LUSO-BRASILEIRO DE RMN, SETEMBRO 23-26 2003, SINTRA, PORTUGAL, (1 PÁGINA)

A SOLID STATE NMR AND RAMAN SPECTROSCOPY STUDY OF GLUCOSE AND MALTOSE
ROSA A, HILLIOU L, AMADO AM, RIBEIRO-CLARO PJA, BROWN SP, GIL AM
5TH INTERNATIONAL MEETING OF THE PORTUGUESE CARBOHYDRATE GROUP,
COVILHÃ, 7-10 SEPTEMBER 2003

ADVANCED HYBRID MATERIALS DOPED WITH MONO-, DI- AND TRIVALENT TRIFLATE SALTS
NUNES S C, BERMUDEZ DE ZEA V, SILVA M M, BARROS S, SMITH M J, SÁ FERREIRA R A, CARLOS L D, ROCHA J
EUROPEAN CONGRESS ON ADVANCED MATERIALS AND PROCESSES, LAUSANNE, SUIÇA (2003)

APPLICATION OF FTIR SPECTROSCOPY FOR THE QUANTIFICATION OF SUGARS IN MANGO JUICE AS A FUNCTION OF RIPENING, IOLA F. DUARTE, ANTÓNIO BARROS, IVONNE DELGADILLO AND ANA M. GIL, 6º ENCONTRO DE QUÍMICA DE ALIMENTOS,

JUNHO 2003, LISBOA. VOLUME I, PP 454-458.

AZA- VERSUS THIO-MACROCYCLIC TRANSITION METAL COMPLEXES: A COMPARATIVE STUDY BY ELECTROSPRAY MASS SPECTROMETRY
MIRANTE FIS; QUINTAL S; MADUREIRA J; FÉLIX V; SANTOS TM;
SANTANA-MARQUES MG
BOOK OF ABSTRACTS OF THE VII FIGIPS MEETING IN INORGANIC CHEMISTRY
2003, 11-14 JUNE PORTUGAL, LISBOA, P 308

β -CYCLODEXTRIN INCLUSION OF SODIUM NIMESULIDE AND PRECURSORS
BRAGA S S; RIBEIRO-CLARO P; PILLINGER M; GONÇALVES I S; PEREIRA F; FERNANDES A C; ROMÃO C C; CORREIA P B; TEIXEIRA-DIAS J J C
7th FGIPS MEETING IN INORGANIC CHEMISTRY
LISBOA, PORTUGAL, 2003. (P 172)

β -CYCLODEXTRIN: PRESPECTIVES OF STUDY
JOSÉ J. C. TEIXEIRA-DIAS, SÉRGIO LIMA, LUÍS CUNHA-SILVA AND CRISTIANO DIAS
“ I JORNADAS DO CICECO”
AVEIRO, PORTUGAL, 19 E 20 DE DEZEMBRO DE 2003

CARBOHYDRATE-DERIVED CHLORINATED COMPOUNDS IN ECF BLEACHING OF HARDWOOD KRAFT PULPS: FORMATION, BEHAVIOUR AND CONTRIBUTION TO AOX IN A BLEACHED KRAFT PULP MILL.,FREIRE, C.S.R., SILVESTRE, A.J.D., PASCOAL NETO, C., SILVA, A.M.S., EVTUGUIN, D.V. AND CAVALEIRO, J.AS., 28TH EUCEPA CONFERENCE, PROCEEDINGS BOOK, P. 292-294, LISBON, PORTUGAL, 2003

CATALYTIC OXIDATION IN POROUS REACTION MEDIA
VALENTE A A; PILLINGER M; NUNES C D; GONÇALVES I S; BRANDÃO P; FERREIRA A; ROCHA J
1^{AS} JORNADAS CICECO, AVEIRO, 2003. (P39)

CELLULOSE PRECURSOR SYNTHESIS OF CERIA-CONTAINING SOFC ANODES
TSIPIS E V; BASHMAKOV I A; KHARTON V V; NAUMOVICH E N; FRADE J R
ABSTRACTS OF THE OSSEP WORKSHOP "IONIC AND MIXED CONDUCTORS: METHODS AND PROCESSES"
2003, AVEIRO, P 34

CELLULOSE/SILICA HYBRIDS PREPARED BY CATALYTIC SOL-GEL PROGRESS. PORTUGAL, I., MAGINA, S., BATISTA, M.A. AND EVTUGUIN D.V. PROCEEDINGS OF 4TH EUROPEAN CONGRESS OF CHEMICAL ENGINEERING, SEPT. 21-25, GRANADA, SPAIN, P. 10.1-002 (2003).

CELLULOSE/SILICA HYBRIDS PREPARED BY A CATALYTIC SOL-GEL PROCESS. I. PORTUGAL, S. SEQUEIRA, S. MAGINA, M.A. BATISTA, D. EVTUGUIN; COMUNICAÇÃO ORAL, 4TH EUROPEAN CHEMICAL ENGINEERING CONFERENCE, GRANADA – SPAIN (2003) O-10.1.002 BOOK OF ABSTRACTS (CD-ROM).

CERAMICS IN VITRO MINERALIZATION PROTOCOLS: A SUPERSATURATION PROBLEM, MARQUES P A A P, MAGALHÃES M C F, CORREIA R.N, MARTIN A I, SALINAS A J, VALLET-REGÍ M
BIOCERAMICS – 16, PROCEEDINGS OF THE 16TH INTERNATIONAL SYMPOSIUM ON CERAMICS IN MEDICINE AND THE ANNUAL MEETING OF THE INTERNATIONAL SOCIETY FOR CERAMICS IN MEDICINE, PORTO, PORTUGAL, 6-9 NOVEMBRO 2003
LIVRO DE RESUMOS, P143, SEM PÁGINAS NUMERADAS

CHANGES IN E. GLOBULUS XYLAN STRUCTURE DURING KRAFT PULPING. PINTO, P. C.O.R., EVTUGUIN D.V., PASCOAL NETO C. BOOK OF ABSTRACTS OF 12TH EUROPEAN CARBOHYDRATE SYMP. (EUROCARB), JULY 6-11, GRENOBLE, FRANCE, P. 136 (2003).

CHANGES IN E. GLOBULUS XYLAN STRUCTURE DURING THE ACID SULPHITE PULPING AND PEROXIDE BLEACHING., EVTUGUIN, D.V. AND GOODFELLOW B.J., BOOK OF ABSTRACTS OF 12TH EUROPEAN CARBOHYDRATE SYMP. (EUROCARB), JULY 6-11, GRENOBLE, FRANCE, P.484 (2003).

CHARACTERISATION OF ACETYLATED XYLO-OLIGOSACCHARIDES FROM EUCALYPTUS GLOBULUS WOOD USING ELECTROSPRAY MASS SPECTROMETRY. PINTO, P.C., REIS, A., EVTUGUIN, D.V., DOMINGUES R. M. AND PASCOAL NETO C. PROCEEDINGS OF 5TH INTERNATIONAL MEETING OF THE PORTUGUESE CARBOHYDRATE GROUP (GLUPOR 5), SEPT. 7-10. COVILHÃ, P. 67 (2003).

CHARACTERIZATION STUDIES ON DI-URETHANESIL ORMOLYTES DOPED WITH LITHIUM TRIFLATE
GONÇALVES M C, OSTROVSKII D, BERMUDEZ V DE ZEA, SILVA M M, BARROS S, MORALES E, SÁ FERREIRA R A, CARLOS L D, SMITH M J, ACOSTA J L
FIRST INTERNATIONAL CONGRESS ON POLYMER BATTERIES AND FUEL CELLS, CHEJU ISLAND, KOREA (2003)

CICECO'S STUDIES OF ADVANCED MOLECULAR AND SUPRAMOLECULAR MATERIALS: A BRIEF REPORT
CAVALEIRO, A M V
1^{as} JORNADAS DO CICECO
AVEIRO, 19 E 20 DE DEZEMBRO 2003
LIVRO DE RESUMOS, PP 24-25

COMPARATIVE CYTOTOXICITY STUDIES OF Cp_2MoCl_2 AND THE INCLUSION COMPLEX β -CD- Cp_2MoCl_2

TEIXEIRA L J; BRAGA S S; MARQUES M P M; GONÇALVES I S; TEIXEIRA-DIAS J J C

7th FGIPS MEETING IN INORGANIC CHEMISTRY
LISBOA, PORTUGAL, 2003. (P 221)

COMPARATIVE STUDY OF LIPOPHILIC EXTRACTIVES OF EUCALYPTUS SPECIES AND BETULA VERRUCOSA WOODS. PINTO, P.C., FREIRE, C.S., SILVESTRE, A.J.D., EVTUGUIN, D.V. AND PASCOAL NETO, C. 5^o ENCONTRO NACIONAL DE QUÍMICA ORGANICA (1^o SIMPÓSIO LUSO-JAPONÊS), 1-4 DE JULHO, AVEIRO, P.64 (2003).

COMPARISON OF YEAST RESPONSE TO INCREASED PRESSURE AT AEROBIC AND ANAEROBIC CONDITIONS.
BELO, I., FERREIRA, E.C., PINHEIRO, R., COUTINHO, J.A.P., COELHO, M.A.Z., 11TH EUROPEAN CONGRESS ON BIOTECHNOLOGY. BASEL, SUIÇA, AGOSTO 2003.

COMPÓSITOS FOSFOSILICATOS COM EURÓPIO PARA OBTENÇÃO DE GUIAS DE ONDA,
FILHO F A D, CARLOS L D, ROCHA J, MESSADEQ Y, RIBEIRO S J L
XXVI REUNIÃO ANUAL DA SOCIEDADE BRASILEIRA DE QUÍMICA, POÇOS DE CALDAS, M.G., BRASIL (2003)

COMPUTING TOOLS FOR QUICK INSPECTION AND INTERPRETATION OF IMPEDANCE SPECTRA, ABRANTES J C C, FRADE J R, OSSEP WORKSHOP ON IONIC AND MIXED CONDUCTORS: METHODS AND PROCESSES, AVEIRO, PORTUGAL, APRIL 10-12, 2003

COR E COORDENADAS DE COR
CARLOS L D
ORAL COMMUNICATION: 3^o ENCONTRO NACIONAL DE TERRAS RARAS, INSTITUTO DE QUÍMICA, UNESP, ARARAQUARA, S.P., BRASIL (2003)

CROSS-BRIDGED POLYPYRIDYL RUTHENIUM COMPLEXES: SOLID STATE AND SOLUTION CO-ORDINATION MODES
MADUREIRA J; SANTOS TM; GOODFELLOW BJ; FÉLIX V
BOOK OF ABSTRACTS OF THE VII FIGIPS MEETING IN INORGANIC CHEMISTRY
2003, 11-14 JUNE PORTUGAL, LISBOA, OR 17

CRYSTALLINE INCLUSION COMPOUNDS OF NONIONIC SURFACTANTS (C_NE_M) IN α -CYCLODEXTRIN, AT VARIOUS RELATIVE HUMIDITIES (COMUNICAÇÃO EM CARTAZ)
LUÍS CUNHA-SILVA AND JOSÉ J. C. TEIXEIRA-DIAS
“MOLECULAR CRYSTAL ENGINEERING: EUROCONFERENCE ON DESIGN AND PREPARATION OF MOLECULAR MATERIALS”
AQUAFREDA DE MARATEA, ITÁLIA, 31 DE MAIO A 5 DE JUNHO DE 2003

DEPOSITION/DETACHMENT OF PARTICLES ON PLASMA TREATED POLYMER SURFACES, M .LEHOCKÝ, L. LAPČÍK, JR., M.C. NEVES, T.

TRINDADE, L. SZYK-WARSZYNSKA, P. WARSZYNSKI, D HUI.
THERMEC'2003- INTERNATIONAL CONFERENCE ON PROCESSING AND
MANUFACTURING OF ADVANCED MATERIALS, 7 A 11 DE JULHO (2003),
MADRID, SPAIN.

DESIGN OF RUTHENIUM MACROCYCLIC THIOETHER AND POLYPYRIDYL
COMPLEXES: INTERACTIONS WITH DNA AND DNA MODELS
SANTOS TM; GOODFELLOW BJ; QUINTAL S; PEDROSA DE JESUS JD; FÉLIX
V

LIVRO DE RESUMOS DAS 1^{AS} JORNADAS DO CICECO
2003, 19 DEZEMBRO PORTUGAL, AVEIRO, P14

DETERMINATION OF SYRINGYL:GUAIACYL RATIOS IN LIGNIN BY PY-GS-
MS. XAVIER, A.F., PINTO, P.C., PASCOAL NETO, C., EVTUGUIN, D.V. AND
SILVESTRE, A.J.D 5º ENCONTRO NACIONAL DE QUÍMICA ORGANICA (1º
SIMPÓSIO LUSO-JAPONÊS), 1-4 DE JULHO, AVEIRO, P.66 (2003).

DFT CALCULATIONS ON NEW CYANIDE-BRIDGED POLYNUCLEAR
COMPLEXES OF Mo AND Cr
COSTA P J; CALHORDA M J; FÉLIX V; GAMELAS C A; GONÇALVES I S;
PEREIRA C C L; ROMÃO C C
7th FGIPS MEETING IN INORGANIC CHEMISTRY
LISBOA, PORTUGAL, 2003. (P 200)

DIELECTRIC CHARACTERIZATION OF THE LEAD-FREE RELAXOR
0.9BaTiO₃-0.1La(Mg_{1/2}Ti_{1/2})O₃ CERAMICS, SALAK A.N., SEABRA M.P.,
FERREIRA V.M., VIEIRA L.G., RIBEIRO J.L., 10TH EUROPEAN MEETING ON
FERROELECTRICITY (EMF 2003) - CAMBRIDGE, UK, J. CONF. ABSTR., 8
(2003) 289.

DIELECTRIC STUDY OF THE (1-X)La(Mg_{1/2}Ti_{1/2})O₃ - XSrTiO₃ CERAMICS,
SEABRA M.P., SALAK A.N., FERREIRA V.M., VIEIRA L.G., RIBEIRO J.L., 10TH
EUROPEAN MEETING ON FERROELECTRICITY (EMF 2003) - CAMBRIDGE,
UK, J. CONF. ABSTR., 8 (2003) 296.

DYNAMIC RHEOLOGICAL ANALYSIS OF CRYSTALLIZATION-INDUCES
GELATION IN WAXY CRUDE OILS.
LOPES DA SILVA, J.A., COUTINHO, J.A.P.,
AERC 2003, GUIMARÃES, SETEMBRO 2003.

EFFECT OF [CR^V-BT]²⁻ ON LYMPHOID ORGANS THYMUS AND SPLEEN: A
HEALTH PERSPECTIVE
OLIVEIRA H; GOMES A; SANTOS T M; SANTOS C; PEREIRA M L
CICTA 2003, ENVIRONMENTAL PROBLEMS IN AN IBEROAMERICAN
CONTEXT. 5TH IBERIAN CONGRESS AND 2ND IBEROAMERICAN ON
ENVIRONMENTAL CONTAMINATION AND TOXICOLOGY, PORTO, 22 A 24
DE SETEMBRO DE 2003.

EFFECT OF THE ENZYME CONCENTRATION ON THE DIRECT
COAGULATION CASTING OF HYDROXYAPATITE-ALUMINA BODIES

ROLO A; TAVARES A; SENOS A M R; ALMEIDA M
BOOK OF ABSTRACTS, XI ENCONTRO SPM
2003, PP177

EFFECTS OF SINTERING ADDITIVES ON THE MIXED TRANSPORT
PROPERTIES OF CERIA BASED MATERIALS UNDER REDUCING
CONDITIONS
COLL D P, NUÑEZ P, ABRANTES J C C, FRADE J R, OSSEP WORKSHOP ON
IONIC AND MIXED CONDUCTORS: METHODS AND PROCESSES, AVEIRO,
PORTUGAL, APRIL 10-12, 2003

ELECTRICAL PROPERTIES OF $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TlO}_3 - \text{SrTiO}_3$ CERAMICS”, GOMAH-
PETTRY J.R., MARCHET P., SALAK A., FERREIRA V.M., MERCURIO J.P., 10TH
EUROPEAN MEETING ON FERROELECTRICITY (EMF 2003) - CAMBRIDGE,
UK, J. CONF. ABSTR., 8 (2003) 141.

ELECTROCHEMICAL REDUCTION OF COPPER(II) TO COPPER(I) IN
POLYOXOTUNGSTATES
GAMELAS, J A F; BALULA, M S; FONSECA, A P; CARAPUÇA, H M;
CAVALEIRO, A M V
7TH FIGIPS MEETING IN INORGANIC CHEMISTRY
LISBOA, PORTUGAL, 11-14 DE JUNHO, 2003,
BOOK OF ABSTRACTS, P191

ENSAIOS PRÉ-CLÍNICOS SOBRE TOXICIDADE DE METAIS: UM EXEMPLO
DA INTERDISCIPLINARIDADE NA UA
PEREIRA M L
ELEMENTOS INORGÂNICOS NA SAÚDE. TÉCNICAS DE DIAGNÓSTICO
NUMA VISÃO INTERDISCIPLINAR
UA, 25 DE SETEMBRO 2003.

EUROPIUM(III) AND GADOLINIUM(III) TRIS- β -DIKETONATE ADDUCTS
WITH HETEROCYCLIC AMINES
FERNANDES J A; SÁ FERREIRA R A; PILLINGER M; JEPSEN J; HAZELL A;
RIBEIRO-CLARO P; CARLOS L D; GONÇALVES I S
7th FGIPS MEETING IN INORGANIC CHEMISTRY
LISBOA, PORTUGAL, 2003. (P 228)

EUROPIUM DOPED PHOSPHOSILICATE WAVEGUIDES
DIAS FILHO F A, RIBEIRO S J L, GONÇALVES R R, MESSADDEQ Y, CARLOS,
L D, BERMUDEZ DE ZEA V, ROCHA J
5TH INTERNATIONAL CONFERENCE ON F-ELEMENTS, GENEVA, SUIÇA
(2003)

EVALUATION OF THE BIOMINERALIZATION ABILITY OF NOVEL
CHITOSAN/SILICA HYBRIDS
SILVA S S, CARLOS L D, ROCHA J, MANO J F, REIS R L
NATO - ADVANCED STUDY INSTITUTE (ASI): “LEARNING FROM NATURE
HOW TO DESIGN NEW IMPLANTABLE BIOMATERIALS: FROM

BIOMINERALIZATION FUNDAMENTALS TO BIOMIMETIC MATERIALS AND PROCESSING ROUTES”, ALVOR, PORTUGAL (2003)

EVIDENCE OF C-H...O INTERMOLECULAR INTERACTIONS WITH LESS USUAL ACCEPTOR GROUPS: THE METHYL TRIOXORHENIUM CASE
VAZ P; RIBEIRO CLARO P J A
PROCEEDINGS OF THE 7TH FIGIPS, LISBON, 11-14 JUNE 2003

FERRIHYDRITE ANTIFERROMAGNETIC NANOPARTICLES ANCHORED IN AN ORGANIC-INORGANIC MATRIX
SILVA N J O, AMARAL V S, CARLOS L D, BERMUDEZ DE ZEA V
INTERNATIONAL CONFERENCE ON MAGNETISM, ICM 2003, ROMA, ITÁLIA (2003)

FERROELECTRIC DOMAIN STRUCTURE AND LOCAL PIEZOELECTRIC PROPERTIES OF SOL-GEL DERIVED $PB(ZR_{1-x}TI_x)O_3$ FILMS, I. K. BDIKIN, V. V. SHVARTSMAN, S-H. KIM, A. L. KHOLKIN
ABSTRACTS OF THE MATERIALS RESEARCH SOCIETY MEETING, SYMPOSIUM C: FERROELECTRIC THIN FILMS XII
DEC. 2-5 2003, BOSTON, USA, P. 63

FERROELECTRIC DOMAIN STRUCTURE OF PZT THIN FILMS WITH DIFFERENT COMPOSITIONS STUDIED BY SPM, A.WU, P. M. VILARINHO, A. L. KHOLKIN, I. M. MIRANDA SALVADO
ABSTRACTS OF THE MATERIALS RESEARCH SOCIETY MEETING, SYMPOSIUM C: FERROELECTRIC THIN FILMS XII DEC. 2-5 2003, BOSTON, USA, P. 85

FERROELECTRIC PROPERTIES OF $BATIO_3$ DOPED WITH $LA(MG_{1/2}TI_{1/2})O_3$, SALAK A.N., SHVARTSMAN V.V., SEABRA M.P., KHOLKIN A.L., FERREIRA V.M., 10TH EUROPEAN MEETING ON FERROELECTRICITY (EMF 2003) - CAMBRIDGE, UK, J. CONF. ABSTR., **8** (2003) 289.

FLOW CITOMETRY AS A TOOL TO EVALUATE MALE INFERTILITY IN CITOTOXIC ASSAYS: AN APPLICATION TO HEAVY METAL TOXICITY
OLIVEIRA H; LOUREIRO J; PEREIRA M L BIOTEC 2003, LISBOA 6-8 DEZEMBRO.

FORMATION OF FERRIHYDRITE NANOPARTICLES IN A SOL-GEL DERIVED ORGANIC-INORGANIC HYBRID MATRIX
SILVA N J O, AMARAL V S, CARLOS L D, ROCHA J, BERMUDEZ DE ZEA V
EUROPEAN CONGRESS ON ADVANCED MATERIALS AND PROCESSES, LAUSANNE, SUIÇA (2003)

FREQUENCY-DEPENDENT ELECTROMECHANICAL RESPONSE IN FERROELECTRIC MATERIALS MEASURED VIA PIEZORESPONSE FORCE MICROSCOPY, I. K. BDIKIN, V. V. SHVARTSMAN, S-H. KIM, A. L. KHOLKIN
ABSTRACTS OF THE MATERIALS RESEARCH SOCIETY MEETING, SYMPOSIUM C: FERROELECTRIC THIN FILMS XII, DEC. 2-5 2003, BOSTON, USA, P. 84.

FUNCTIONAL ASPECTS OF BULK AND INTERFACIAL GALACTOMANNAN-WHEY PROTEIN INTERACTIONS, S. CARNEIRO, C. TAVARES, S. R. MONTEIRO, A. B. TIMMONS & J. A. LOPES DA SILVA, X CONGRESSO NACIONAL DE BIOTECNOLOGIA, LISBON (PORTUGAL), 6 - 8 DECEMBER 2003.

FUNCTIONAL INORGANIC/POLYMER NANOCOMPOSITES, A. BARROS TIMMONS, A.C. ESTEVES, T. TRINDADE, 1^a JORNADAS DO CICECO, AVEIRO (PORTUGAL), 19-20 DECEMBER.

GAS SOLUBILITY IN NATURAL AND BIODEGRADABLE POLYMERS FOR FOOD PACKAGING.

COUTINHO, J.A.P., OLIVEIRA, N.S., BARROS, A., DARIDON, J.L., MARRUCHO, I.M.,
THERMODYNAMICS POLISH-FRENCH DAYS, NOVEMBER 2003.

GAS SOLUBILITY IN POLYMER NANOCOMPOSITES, N. S. OLIVEIRA, A. C. ESTEVES, A. BARROS, T. TRINDADE, J. A. P. COUTINHO, A. FERREIRA, I. M. MARRUCHO, 20TH ESAT: EUROPEAN SYMPOSIUM ON APPLIED THERMODYNAMICS, LAHNSTEIN (GERMANY), 8-12 OCTOBER, 2003.

GROWTH KINETICS OF $\text{SrBi}_2\text{Ta}_2\text{O}_9$ SINGLE CRYSTALS BY SEEDED POLYCRYSTALLINE CONVERSION, H. AMORIN, M. COSTA, A. L. KHOLKIN ABSTRACTS OF THE 10TH EUROPEAN MEETING ON FERROELECTRICITY, CAMBRIDGE, UK, 3-8 AUG, 2003, J. OF CONF. ABS. 8. P. 60 (2003).

HETERONUCLEAR CORRELATIONS INVOLVING QUADRUPOLAR NUCLEI, A THROUGH BOND APPROACH USING J-COUPPLINGS
MASSIOT D; FAYON F; ALONSO B; MONTOUILLOUT V; FERNANDEZ C;
MORAIS C AND ROCHA J
3RD ALPINE CONFERENCE, ON SOLID-STATE NMR CHAMONIX MONT-BLANC, FRANCE, SEPTEMBER 14-18, 2003.

HIGH RESOLUTION NMR AND DIFFUSION-ORDERED SPECTROSCOPY OF PORT WINE, MATHIAS L. NILSSON, CLÁUDIA ALMEIDA, IOLA DUARTE, IVONNE DELGADILLO, GARETH A. MORRIS AND ANA M. GIL, SMASH 2003, SMALL MOLECULE NMR CONFERENCE, SETEMBRO 14-17, 2003, VERONA, ITÁLIA, (1 PÁGINA)

HIGH RESOLUTION NMR AND DIFFUSION-ORDERED SPECTROSCOPY OF PORT WINE, MATHIAS L. NILSSON, CLÁUDIA ALMEIDA, IOLA DUARTE, IVONNE DELGADILLO, GARETH A. MORRIS AND ANA M. GIL, II ENCONTRO LUSO-BRASILEIRO DE RMN, SETEMBRO 23-26 2003, SINTRA, PORTUGAL, (2 PÁGINAS)

HOW STRONG ELECTROLYTES AFFECT THE INCLUSION OF DECANOIC ACID IN β -CYCLODEXTRIN (COMUNICAÇÃO EM CARTAZ)
SÉRGIO LIMA, BRIAN J. GOODFELLOW, JOSÉ J. C. TEIXEIRA-DIAS
"MOLECULAR LIQUIDS: ROUTES FROM LOCAL ORDER TO LARGE-SCALE COOPERATIVITY EUROCONFERENCE"

CASTELVECCHIO PASCOLI, ITÁLIA, 5-10 DE SETEMBRO DE 2003

HOW STRONG ELECTROLYTES AFFECT THE INCLUSION OF DECANOIC ACID IN β -CYCLODEXTRIN (COMUNICAÇÃO EM CARTAZ)

SÉRGIO LIMA, BRIAN J. GOODFELLOW, JOSÉ J. C. TEIXEIRA-DIAS

“II ENCONTRO LUSO-BRASILEIRO DE RMN”

SINTRA, PORTUGAL, 23-26 DE SETEMBRO DE 2003

IMMOBILISATION OF METALLO-ORGANIC SPECIES IN LAYERED DOUBLE HYDROXIDES

PILLINGER M; GAGO S; GONÇALVES I S; SANTOS T M; ROCHA J

1^{AS} JORNADAS CICECO, AVEIRO, 2003. (O PG. 15)

IMPORTÂNCIA BIOLÓGICA DE COMPOSTOS DE CRÓMIO: UM CASO DE ESTUDO

SANTOS TM

LIVRO DE RESUMOS DO SEMINÁRIO: ELEMENTOS INORGÂNICOS NA SAÚDE: TÉCNICAS DE DIAGNÓSTICO NUMA VISÃO INTERDISCIPLINAR 2003, 25 SETEMBRO, PORTUGAL, AVEIRO, P 5-6

IN SITU EMULSION POLYMERIZATION OF $Bi_2S_3@SiO_2/POLY(STYRENE)$ NANOCOMPOSITES, ESTEVES, A.C.; NEVES, M.C.; BARROS-TIMMONS, A.; TRINDADE, T.; BOURGEAT-LAMI, E.; LIZ-MARZÁN, L.; MACROMOLECULES 2003-NATO ASI. PISA (ITALY), 6-15 OCTOBER 2003.

INCLUSION COMPOUNDS FORMED BETWEEN LUMINESCENT LANTHANIDE COMPLEXES AND CYCLODEXTRINS

GONÇALVES I S; FERNANDES J A; BRAGA S S; SÁ FERREIRA R A; PILLINGER M; CARLOS L D; RIBEIRO-CLARO P

1^{AS} JORNADAS CICECO, AVEIRO, 2003. (P8)

INFLUENCE OF INTERFACIAL PARAMETERS ON THE PROPERTIES OF $SiO_2/POLY(STYRENE)$ NANOCOMPOSITES, ESTEVES, A.C.; BARROS-TIMMONS, A.; LAPCIK, L.J.; TRINDADE, T.; MACROMOLECULES 2003-NATO ASI. PISA (ITALY), 6-15 OCTOBER 2003.

INFLUENCE OF PREPARATION CONDITIONS ON STRUCTURE AND MAGNETIC PROPERTIES OF SOL-GEL DERIVED IRON-DOPED SILOXANE-POLY(ETHYLENE OXIDE) NANOCOMPOSITES

PULCINELLI S H, SILVA N J O, CARLOS L D, AMARAL V S, CHIAVACCI L A, DAHMOUCHE K, SANTILLI C V, BRIOIS V, CRAIEVICH A F
ORAL COMMUNICATION: XI INTERNATIONAL WORKSHOP ON GLASSES, CERAMICS, HYBRIDS AND NANOCOMPOSITES FROM GELS, SYDNEY, AUSTRÁLIA, (2003)

INFLUENCE OF THE ATMOSPHERIC MOISTURE ON THE CONDUCTIVITY OF LAYERED SODIUM CATION CONDUCTORS $Na_x(M_yL_{1-y})O_2$ (M = NI, FE; L = TI, SB)

SMIRNOVA O A; KHARTON V V; MARQUES F M B

ABSTRACTS OF THE 5TH IBEROAMERICAN CONFERENCE
"ELECTROCERÁMICA" (CD ROM)
2003, SPAIN, P 43

INFLUÊNCIA DA ADIÇÃO DE CINZAS PESADAS DE CARVÃO MINERAL
NAS PROPRIEDADES MECÂNICAS E FÍSICAS DE MATERIAIS CERÂMICOS
KNISS C; SEGADÃES A M; KUHNEN NC; RIELLA HG; HOTZA D; ACCHAR
W
RESUMOS DO 47º CONGRESSO BRASILEIRO DE CERÂMICA, JOÃO PESSOA-
PB, BRASIL, JUNHO 2003 (REF:6-17).

INSERTION OF IRON OXIDE IN CALCIUMSILICATE GEL-DERIVED
MATERIALS - M.G. FERREIRA DA SILVA AND J.C. WAERENBORGH
APRESENTADA NO COLLOQUIM SPECTROSCOPICUM INTERNATIONAL
XXXIII REALIZADO EM GRANADA EM SETEMBRO DE 2003.

INTERACTION OF RUTHENIUM COMPLEXES WITH DNA MODELS: AN
NMR STUDY (COMUNICAÇÃO EM CARTAZ)
SUSANA QUINTAL, TERESA M. SANTOS, BRIAN J. GOODFELLOW AND
VITOR FÉLIX
"II ENCONTRO LUSO-BRASILEIRO DE RMN"
SINTRA, PORTUGAL, 23-26 DE SETEMBRO DE 2003

INVESTIGATION OF DOMAIN STRUCTURE OF $\text{SRBI}_2\text{TA}_2\text{O}_9$ SINGLE
CRYSTALS BY POLARIZED OPTICAL AND PIEZOELECTRIC FORCE
MICROSCOPY
H. AMORIN, V. SHVARTSMAN, M. E. V. COSTA, A. L. KHOLKIN, J.-P.
MERCURIO, G. TROLLARD, M. MANIER
ABSTRACTS OF THE 10TH EUROPEAN MEETING ON FERROELECTRICITY,
CAMBRIDGE, UK, 3-8 AUG, 2003, J. OF CONF. ABS. 8. P. 60 (2003).

INVESTIGATION OF NOVEL ORMOLYTES FOR SOLID STATE MAGNESIUM
BATTERIES
NUNES S C, BERMUDEZ DE ZEA V, SILVA M M, BARROS, SÁ FERREIRA R
A, CARLOS L D, ROCHA J, SMITH M. J
54TH ANNUAL MEETING OF THE INTERNATIONAL SOCIETY OF
ELECTROCHEMISTRY, SÃO PEDRO (S. PAULO), BRASIL (2003)

INVESTIGATION OF REACTIVITY OF SOME NOVEL 1,4,7-
TRIAZACYCLONONANE AND 1,1,1-TRIS(AMINOMETHYL)ETHANE
COMPLEXES IN CATALYSIS OF ALKENE EPOXIDATION
PETROVSKI Z; ABRANTES M; GONÇALVES I S; ROYO B; ROMÃO C C
7th FGIPS MEETING IN INORGANIC CHEMISTRY
LISBOA, PORTUGAL, 2003. (P 336)

INVESTIGATION OF REACTIVITY OF SOME NOVEL 1,4,7-
TRIAZACYCLONONANE AND 1,1,1-TRIS(AMINOMETHYL)ETHANE
COMPLEXES IN CATALYSIS OF ALKENE EPOXIDATION
PETROVSKI Z; ABRANTES M; GONÇALVES I S; ROYO B; ROMÃO C C

XVTH FEICHEM CONFERENCE ON ORGANOMETALLIC CHEMISTRY,
ZURIQUE, 2003. (PO 114)

IONIC AND ELECTRONIC TRANSPORT IN FE-CONTAINING APATITE
PHASES

SHAULA A L; KHARTON V V; MARQUES F M B

ABSTRACTS OF THE OSSEP WORKSHOP "IONIC AND MIXED
CONDUCTORS: METHODS AND PROCESSES"

2003, AVEIRO, P 11

IRON-DOPED SILOXANE-POLY(ETHYLENE OXIDE) NANOCOMPOSITES:
RELATIONSHIPS BETWEEN STRUCTURE AND PROPERTIES

CHIAVACCI L A, DAHMOUCHE K, CARLOS L D, AMARAL V S, BERMUDEZ
DE ZEA V, PULCINELLI S H, SANTILLI C V

ORAL COMMUNICATION: X CONFERENCE ON THE PHYSICS OF NON-
CRYSTALLINE SOLIDS, PARMA, ITÁLIA (2003)

KEGGIN-TYPE POLYOXOTUNGSTATES SUBSTITUTED WITH MANGANESE
(III): A COMPARISON STUDY

SANTOS, I C M S; BALULA, M S S; SIMÕES, M M Q; NEVES, M G P M S;
CAVALEIRO, J A S; CAVALEIRO, A M V, SCHLINDWEIN, W

7TH FIGIPS MEETING IN INORGANIC CHEMISTRY

LISBOA, PORTUGAL, 11-14 DE JUNHO, 2003

BOOK OF ABSTRACTS, P408

KEGGIN-TYPE TUNGSTOBORATES IN HOMOGENEOUS OXIDATIVE
CATALYSIS

SANTOS, I C M S; BALULA, M S S; SIMÕES, M M Q; NEVES, M G P M S;
CAVALEIRO, J A S; CAVALEIRO, A M V

6º ENCONTRO DA DIVISÃO DE CATÁLISE E MATERIAIS POROSOS,

ÉVORA, PORTUGAL, 30-31 DE MAIO DE 2003,

LIVRO DE RESUMOS, PP 87-88

LA(MG_{1/2}TI_{1/2})O₃ - BASED MATERIALS FOR MICROWAVE APPLICATIONS,
SEABRA M.P., SALAK A.N., AVDEEV M., FERREIRA V.M., II

INTERNATIONAL MATERIALS SYMPOSIUM (MATERIALS 2003) -

CAPARICA, PORTUGAL, (2003) 54 (P1.12).

LAYER-BY-LAYER ASSEMBLY OF BI₂S₃/SIO₂ AND CDS NANOPARTICLES,

M. C. NEVES, L. M. LIZ-MARZÁN, T. TRINDADE, 7TH FIGIPS MEETING IN
INORGANIC CHEMISTRY, 11-14 JUNHO, LISBOA, (2003); 5ª REUNION

NACIONAL DEL GRUPO ESPECIALIZADO DE COLOIDES E INTERFASES, 3-5
JULHO (2003), VIGO.

LAYERED DOUBLE HYDROXIDES PILLARED BY HETEROCYCLIC AMINES,
S. GAGO, M. PILLINGER, A. A. VALENTE, T. M. SANTOS, J. ROCHA, I. S.

GONÇALVES, 6º ENCONTRO DIVISÃO DE CATÁLISE E MATERIAIS
POROSOS, ÉVORA, 2003.

LIGHT EMISSION AND LOCAL-STRUCTURE OF Eu(III)-BASED AMINE-FUNCTIONALISED ORGANIC/INORGANIC HYBRIDS

CARLOS L D, SÁ FERREIRA R A, GONÇALVES M C, BERMUDEZ DE ZEA V
ORAL COMMUNICATION: 5TH INTERNATIONAL CONFERENCE ON F-ELEMENTS, GENEVA, SUIÇA (2003)

LIGHT EMISSION OF Eu (III)-DOPED MICROPOROUS Ti, Zr AND Hf SILICATES

RAINHO J P; ANANIAS D; LIN Z; CARLOS L D AND ROCHA J
5TH INTERNATIONAL CONFERENCE ON F-ELEMENTS ICFE'5, GENEVA, SWITZERLAND, AUGUST 24-29, 2003, P. 123, PC-65.

LIPOPHILIC EXTRACTIVES OF ACACIA MANGIUM WOOD. FREIRE, C.S., SILVESTRE, A.J.D., PINTO, P.C., PASCOAL NETO, C. AND EVTUGUIN, D.V. 5º ENCONTRO NACIONAL DE QUÍMICA ORGANICA (1º SIMPÓSIO LUSO-JAPONÊS), 1-4 DE JULHO, AVEIRO, P.65 (2003).

LITERACIA CIENTÍFICA VERSUS UM CASO DE ENVENAMENTO POR CO SARAIVA AP; SANTOS TM

LIVRO DE RESUMOS DO III ENCONTRO DEDQ, A QUÍMICA E OS NOVOS DESAFIOS DA COMUNICAÇÃO (SOCIEDADE PORTUGUESA DE QUÍMICA) 2003, 20-21 NOVEMBRO PORTUGAL, PÓVOA DO VARZIM, P-1

LOCAL ELECTROMECHANICAL PROPERTIES OF FERROELECTRIC RELAXORS STUDIED BY PIEZORESPONSE FORCE MICROSCOPY, A. KHOLKIN, V. SHVARTSMAN, M. WOITAS, J. SALDAÑA, S. VAKHRUSHEV, A. SAFARI,

ABSTRACTS OF THE 10TH EUROPEAN MEETING ON FERROELECTRICITY, CAMBRIDGE, UK, 3-8 AUG, 2003, J. OF CONF. ABS. 8. P. 181 (2003).

LOCAL ELECTROMECHANICAL PROPERTIES OF PBMG173NB2/3O3 THIN FILMS STUDEIED BY PIEZOELECTRIC FORCE MICROSCOPY, V.

SHVARTSMAN, M. TYUNINA, J. LEVOSKA, A. KHOLKIN,
ABSTRACTS OF THE 10TH EUROPEAN MEETING ON FERROELECTRICITY, CAMBRIDGE, UK, 3-8 AUG, 2003, J. OF CONF. ABS. 8. P. 309 (2003).

LUMINESCENT PROPERTIES OF LANGMUIR-BLODGETT FILMS BASED ON AN EUROPIUM-POLYOXOTUNGSTATE ANION

SOUSA, F; FERREIRA, A; FERREIRA, R; CAVALEIRO, A V; CARLOS, L D; NOGUEIRA, H I S; TRINDADE, T
5TH CONFERENCE ON F-ELEMENTS, ICFE'5, GENEVA, SUIÇA, 24-29 DE AGOSTO, 2003, BOOK OF ABSTRACT, PP176

MAGNETIC FERRIHYDRITE NANOPARTICLES DISPERSED IN AN HYBRID MATRIX

SILVA N J O, AMARAL V S, CARLOS L D, BERMUDEZ DE ZEA V
ORAL COMMUNICATION: 2003 SPRING MEETING OF THE MATERIALS RESEARCH SOCIETY, NANOMAGNETISM, S. FRANCISCO, EUA (2003)

MALE GERM CELLS AS TARGETS FOR HEAVY METALS: IMPLICATIONS ON FERTILITY POTENTIAL

COSTA F G; OLIVEIRA H; PEREIRA M L

CICTA 2003, ENVIRONMENTAL PROBLEMS IN AN IBEROAMERICAN CONTEXT. 5TH IBERIAN CONGRESS AND 2ND IBEROAMERICAN ON ENVIRONMENTAL CONTAMINATION AND TOXICOLOGY, PORTO, 22 A 24 DE SETEMBRO DE 2003.

MCM-41 SURFACE-FIXED MO^{VI} ACTIVE SPECIES FOR THE LIQUID-PHASE OXIDATION OF ALCOHOLS, A. A. VALENTE, C. D. NUNES, M. PILINGER, J. ROCHA, I. S. GONÇALVES, 6^º ENCONTRO DIVISÃO DE CATÁLISE E MATERIAIS POROSOS, ÉVORA, 2003.

MESOPOROUS SILICA DERIVATISED WITH BIS(HALOGENO) DIOXOMOLYBDENUM(VI) COMPLEXES, C. D. NUNES, A. A. VALENTE, M. PILLINGER, J. ROCHA, I. S. GONÇALVES, 6^º ENCONTRO DIVISÃO DE CATÁLISE E MATERIAIS POROSOS, ÉVORA, 2003.

METHODS OF INVESTIGATION OF MECHANISMS OF CHROLIUM AND CADMIUM TOXICITY

PEREIRA M L; SANTOS T M

1^ªAS JORNADAS CICECO, UA 19-20 DEZEMBRO 2003.

MICROSTRUCTURAL DEVELOPMENT IN HIGH-QUALITY PZT THIN FILMS PREPARED BY SOL-ROUTE AT LOW TEMPERATURE, J. PEREZ, P.M.

VILARINHO, A. L. KHOLKIN

ABSTRACTS OF THE 10TH EUROPEAN MEETING ON FERROELECTRICITY, CAMBRIDGE, UK, 3-8 AUG, 2003, J. OF CONF. ABS. 8. P. 259 (2003).

MICROSTRUCTURE AND ELECTRICAL PROPERTIES OF SRBI₂TA₂O₉ CERAMICS PROCESSED BY TEMPLATED GRAIN GROWTH, H. AMORÍN, M.E.V. COSTA AND A. L. KHOLKIN

ABSTRACTS OF THE 2ND INTERNATIONAL MATERIALS SYMPOSIUM, COSTA DE CAPARICA, 14-16 APR. 2003

MIXED CONDUCTING MEMBRANE MATERIALS FOR PARTIAL OXIDATION OF HYDROCARBONS.

FRADE J R; KHARTON V V; MARQUES F M B; TSIPIS E; SHAULA A; YAREMCHENKO A; VYSHATKO N

ABSTRACTS OF THE 5TH IBEROAMERICAN CONFERENCE "ELECTROCERÁMICA" (CD ROM), 2003, SPAIN, P 41

MOLECULAR MODELLING ACROSS THE CHEMISTRY: AB INITIO AND MOLECULAR DYNAMIC SIMULATIONS

FELIX V, RIBEIRO-CLARO P J A, FONSECA N

I JORNADAS CICECO, AVEIRO, 19 E 20 DE DEZEMBRO DE 2003

MOLECULAR STRUCTURE-ACTIVITY RELATIONSHIPS FOR THE OXIDATION OF ORGANIC COMPOUNDS USING MESOPOROUS SILICA CATALYSTS DERIVATIZED WITH BIS (HALOGENO) DIOXOMOLYBDENUM

(VI) COMPLEXES, A. A. VALENTE, C. D. NUNES, M. PILLINGER, J. ROCHA, AND I. S. GONÇALVES, EUROPACAT VI, AUSTRIA, 2003.

MOLECULAR STRUCTURE OF SUPPORTED CATALYSTS DERIVED FROM BIS(HALOGENO)DIOXOMOLYBDENUM(VI) COMPLEXES, C. D. NUNES, A. A. VALENTE, M. PILLINGER, J. ROCHA, I. S. GONÇALVES, 7TH FIGIPS MEETING IN INORGANIC CHEMISTRY, LISBOA, JUNHO, 2003.

MULTIVARIATE ANALYSIS OF FTIR AND NMR DATA OF BEER AS A POTENTIAL TOOL FOR ITS QUALITY CONTROL, CLÁUDIA ALMEIDA, IOLA F. DUARTE, ANTÓNIO BARROS AND ANA M. GIL, 6º ENCONTRO DE QUÍMICA DE ALIMENTOS, JUNHO 2003, LISBOA. VOLUME I, PP 424-427. (4 PÁGINAS)

MULTIVARIATE ANALYSIS OF NMR AND FTIR DATA OF BEER AS A POTENTIAL TOOL FOR ITS QUALITY CONTROL, CLÁUDIA ALMEIDA, IOLA F. DUARTE, ANTÓNIO BARROS AND ANA M. GIL, II ENCONTRO LUSO-BRASILEIRO DE RMN, SETEMBRO 23-26 2003, SINTRA, PORTUGAL, (2 PÁGINAS)

NANOSCALE CHARACTERIZATION AND LOCAL ELECTROMECHANICAL PROPERTIES OF FERROELECTRIC FILMS FOR MEMS
A. L. KHOLKIN, V. V. SHVARTSMAN, A. YU. EMELYANOV, AND A. SAFARI
ABSTRACTS OF THE ELECTROCHEMICAL SOCIETY MEETING, SYMPOSIUM "DIELECTRICS IN EMERGING TECHNOLOGIES", 29 APR – 2 MAY, 2003, PARIS (FRANCE), P.186.

NANOSCALE CHARACTERIZATION AND LOCAL ELECTROMECHANICAL PROPERTIES OF FERROELECTRIC FILMS FOR MEMS, A. KHOLKIN, A. EMELYANOV, V. SHVARTSMAN
ABSTRACTS OF POLECEP WORKSHOP "ADVANCED CHARACTERIZATION OF FERROELECTRIC MATERIALS", CAPRI, ITALY, JUNE 2003.

NANOSCALE FERROELECTRIC PROPERTIES OF PZN-PT SINGLE CRYSTALS STUDIED BY SCANNING FORCE MICROSCOPY, I. K. BDIKIN, V. V. SHVARTSMAN, A. L. KHOLKIN
ABSTRACTS OF THE MATERIALS RESEARCH SOCIETY MEETING, SYMPOSIUM D: MATERIALS AND DEVICES FOR SMART SYSTEMS, DEC. 2-5 2003, BOSTON, USA, P. 105

NANOSCALE INVESTIGATION OF POLAR STRUCTURE OF (1-X)PBMG_{1/3}NB_{2/3}O₃-XPBTIO₃ SINGLE CRYSTALS, V. V. SHVARTSMAN, M. WOJTAS, S. VAKHRUSHEV, A. L. KHOLKIN
ABSTRACTS OF THE MATERIALS RESEARCH SOCIETY MEETING, SYMPOSIUM D: MATERIALS AND DEVICES FOR SMART SYSTEMS, DEC. 2-5 2003, BOSTON, USA, P. 103

NEW AND TRADITIONAL TECHNIQUES TO EVALUATE TOXIC EFFECTS OF HEAVY METALS

OLIVEIRA H; SANTOS C; SANTOS T M; CASCALHEIRA J C; LOPES J C;
MENDIRATTA S K; PEREIRA M L BIOTEC 2003, LISBOA 6-8 DEZEMBRO.

NEW GLASSES - NEW COMPOSITIONS – NEW APPLICATIONS – M.G.
FERREIRA DA SILVA, M.P.F. GRAÇA AND M.A. VALENTE
APRESENTADA NAS 1^{as} JORNADAS CICECO EM DEZEMBRO DE 2003.

NMR STUDIES OF 5-AMINOLEVULINIC ACID SYNTHASE: THE FIRST
ENZYME OF THE HEME BIOSYNTHETIC PATHWAY (COMUNICAÇÃO EM
CARTAZ)

JORGE S DIAS, GLÓRIA C FERREIRA, PETER HENKLEIN, VICTOR WRAY,
ANJOS L MACEDO AND BRIAN J GOODFELLOW
“II ENCONTRO LUSO-BRASILEIRO DE RMN”

NOVEL LARGE-PORE FRAMEWORK TITANIUM SILICATE CATALYST, P.
BRANDÃO, A. A. VALENTE, A. PHILIPPOU, A. FERREIRA, M. ANDERSON, J.
ROCHA, 6^o ENCONTRO DIVISÃO DE CATÁLISE E MATERIAIS POROSOS,
ÉVORA, 2003.

NOVEL LUMINESCENT LANTHANIDE SILICATES

ROCHA J ; CARLOS L D; ANANIAS D ; RAINHO J; LIN, Z AND FERREIRA A
7th FIGIPS MEETING IN INORGANIC CHEMISTRY, FACULDADE DE
CIÊNCIAS, UNIVERSIDADE DE LISBOA, LISBOA, PORTUGAL, JUNE 11-14,
2003, BOOK OF ABSTRACTS, P. 92.

NOVEL LUMINESCENT MATERIALS BASED ON A Eu(III) COMPLEX OF
2,6-DIHYDROXYBENZOIC ACID, AND THE CRYSTAL STRUCTURE OF
[¹⁵Bu₄N]₂[Eu(2,6-HDHB)₅(H₂O)₂]

SOARES-SANTOS P. C. R. , NOGUEIRA H. I. S. , ALMEIDA PAZ F. A. , SÁ
FERREIRA R. A., CARLOS L. D., KLINOWSKI J., TRINDADE T.

5TH INTERNATIONAL CONFERENCE ON F-ELEMENTS, GENEVRA, SUIÇA,
2003.

NOVEL MICROPOROUS AND LAYERED LUMINESCENT LANTHANIDE
SILICATES

ROCHA J; CARLOS L D ; FERREIRA A ; RAINHO J AND ANANIAS D
II INTERNATIONAL MATERIALS SYMPOSIUM AND XI ENCONTRO DA
SOCIEDADE PORTUGUESA DE MATERIAIS, CAMPUS DA CAPARICA,
UNIVERSIDADE NOVA DE LISBOA, PORTUGAL, APRIL 14-16, 2003,
BOOK OF ABSTRACTS, P. 190.

NOVEL MICROPOROUS PHOTOLUMINESCENT RARE-EARTH SILICATES

ROCHA J; CARLOS LD; ANANIAS D AND RAINHO J
SIXTH INTERNATIONAL CONFERENCE ON MATERIALS CHEMISTRY, MC6:
FRONTIERS AND INTERFACES, UNIVERSITY OF SHEFFIELD, UK, JULY 29-
AUGUST 1, 2003, BOOK OF ABSTRACTS, P. CC2.

NOVEL ORMOLYTES FOR LITHIUM BATTERIES

NUNES S C, BERMUDEZ V. DE ZEA, OSTROVSKII D, SILVA M M, BARROS S, SMITH M J, SÁ FERREIRA R A, CARLOS L D, ROCHA J
FIRST INTERNATIONAL CONGRESS ON POLYMER BATTERIES AND FUEL CELLS, CHEJU ISLAND, KOREA (2003)

OLIMPIADAS DE QUÍMICA: UMA OPORTUNIDADE PARA O ENSINO E DIVULGAÇÃO DA QUÍMICA
RIBEIRO CLARO P J A
ORAL PRESENTATION
III ENCONTRO DA DIVISÃO DE ENSINO E DIVULGAÇÃO DA QUÍMICA
PÓVOA DE VARZIM, 20-21 NOVEMBER 2003

OPTIMISATION OF LACCASE PRODUCTION BY TRAMETES VERSICOLOR IN BIOREACTOR.
TAVARES, A.P.M., COUTINHO, J.A.P., XAVIER, A.M.B.R., COELHO, M.A.Z., EUROPEAN CONFERENCE OF CHEMICAL ENGINEERING, GRANADA, ESPANHA, SETEMBRO 2003.

OPTIMIZAÇÃO DAS CONDIÇÕES DO MEIO DE CULTURA PARA A PRODUÇÃO DE EXO-BIOPOLÍMERO POR TRAMETES (CORIOLUS) VERSICOLOR.
AGAPITO, M.S.M., TAVARES, A.P.M., LOPES DA SILVA, J.A., BARROS.TIMMONS, A., COUTINHO, J.A.P., XAVIER, A.M.R.B., BIOTEC'2003, LISBOA, DEZEMBRO 2003.

ORDERED BENZENE-SILICA HYBRIDS WITH MOLECULAR-SCALE PERIODICITY IN THE WALLS AND DIFFERENT MESOPORE SIZES, P. FERREIRA, N. BION, A. A. VALENTE, I. S. GONÇALVES, J. ROCHA, 6º ENCONTRO DIVISÃO DE CATÁLISE E MATERIAIS POROSOS, ÉVORA, 2003.

ORGANOMETALLIC-ANION-PILLARED LAYERED DOUBLE HYDROXIDES
GAGO S; PILLINGER M; SANTOS T M; ROCHA J; GONÇALVES I S
7th FGIPS MEETING IN INORGANIC CHEMISTRY
LISBOA, PORTUGAL, 2003. (P 237)

OXIDATION OF CYCLOALKANES WITH HYDROGEN PEROXIDE IN THE PRESENCE OF KEGGIN TYPE POLYOXOTUNGSTATES
SIMÕES, M M Q; SANTOS, I C M S; BALULA, M S S; GAMELAS, J A F; CAVALEIRO, A M V; NEVES, M G P M S; CAVALEIRO, J A S
7TH EUROPEAN WORKSHOP MEETING ON SELECTIVE OXIDATION, INNOVATIVE SELECTIVE OXIDATIONS: NANOSCALE AND DYNAMIC ASPECTS (ISO 2003)
INNSBRUCK, ÁUSTRIA, 1-2 DE SETEMBRO DE 2003, POSTER 32

OXIDATION OF CYCLOALKANES WITH H₂O₂ IN THE PRESENCE OF KEGGIN-TYPE POLYOXOTUNGSTOBORATES.
SANTOS, I C M S; BALULA, M S S; SIMÕES, M M Q; NEVES, M G P M S; CAVALEIRO, J A S; CAVALEIRO, A M V
EUROPACAT-VI, INNSBRUCK, AUSTRIA, 31 AGOSTO-4 SETEMBRO, 2003
BOOK OF ABSTRACT B3.194

OXIDATION OF ORGANIC COMPOUNDS WITH H_2O_2 IN THE PRESENCE OF SILICOTUNGSTATES

SIMÕES, M M Q; SANTOS, I C M S; BALULA, M S S; NEVES, M G P M S; CAVALEIRO, J A S; CAVALEIRO, A M V
6º ENCONTRO DA DIVISÃO DE CATÁLISE E MATERIAIS POROSOS, ÉVORA, PORTUGAL, 30-31 DE MAIO DE 2003, LIVRO DE RESUMOS, PP 107-108

ÓXIDO DE VANÁDIO SUPORTADO EM ZEÓLITO NAY E CARVÃO MICROPOROSO: CARACTERIZAÇÃO E APLICAÇÃO EM POLIMERIZAÇÃO DE ETILENO, I. MATOS, Y. ZHANG, I. F. FONSECA, F. LEMOS, M. A. N. D. A. LEMOS, F. FREIRE, A. C. FERNANDES, A. M. BOTELHO DO REGO, A. A. VALENTE, M. M. MARQUES, 6º ENCONTRO DIVISÃO DE CATÁLISE E MATERIAIS POROSOS, ÉVORA, 2003.

ÓXIDO MISTO DE ÍTRIO E ALUMÍNIO OBTIDO PELA METODOLOGIA SOL-GEL NÃO-HIDROLÍTICA, AVILA L R, PEREIRA P F S, DE LIMA O J, CIUFFI K J, MELLO C, CARLOS L D, NASSAR E J
XXVI REUNIÃO ANUAL DA SOCIEDADE BRASILEIRA DE QUÍMICA, POÇOS DE CALDAS, M.G., BRASIL (2003)

OXYGEN NONSTOICHIOMETRY OF $Sr(Co,Fe)O_{3-\delta}$ MIXED CONDUCTORS NAUMOVICH E N; TIKHONOVICH E N; LOGVINOVICH D I; KHARTON V V; SAMOKHVAL V V
ABSTRACTS OF THE OSSEP WORKSHOP "IONIC AND MIXED CONDUCTORS: METHODS AND PROCESSES"
2003, AVEIRO, P 42

OXYGEN PERMEABILITY OF TRANSITION METAL-CONTAINING $La(Sr)Ga(Mg,M)O_{3-\delta}$ CERAMIC MEMBRANES YAREMCHENKO A A; SHAULA A L; KHARTON V V; KOVALEVSKY A A; NAUMOVICH E N; FRADE J R; MARQUES F M B
ABSTRACTS OF THE 5TH IBEROAMERICAN CONFERENCE "ELECTROCERÁMICA" (CD ROM)
2003, SPAIN, P 89

OXYGEN TRANSPORT AND ELECTROCHEMICAL ACTIVITY OF La_2NiO_{4+D} -BASED CATHODE MATERIALS KHARTON V V, YAREMCHENKO A A, TSIPI S E V, FRADE J R, 8TH INT. SYMP. ON SOLID OXIDE FUEL CELLS, APRIL 27-MAY 2, 2003, PARIS, ABSTRACT 1902

PERFLUOROCARBON EMULSIONS: STABILITY AND GAS SOLUBILITY. FREIRE, M.G., DIAS, A.M.A., COELHO, M.A.Z., COUTINHO, J.A.P., MARRUCHO, I.M.
JORGE CALADO: 40 YEARS OF MOLECULAR THERMODYNAMICS, IST, LISBOA, JANEIRO 2003.

PHASE FORMATION, CRYSTAL STRUCTURE AND ELECTRICAL PROPERTIES OF NEW MIXED POTASSIUM ANTIMONATES $K_xM_{(1-x)/3}Sb_{(2-x)/3}O_2$ (M= NI, MG, CO)

SMIRNOVA O A; NALBANDYAN V B; AVDEEV M Y; MEDVEDEVA L I; MEDVEDEV B S; KHARTON V V; MARQUES F M B

ABSTRACTS OF THE 5TH IBEROAMERICAN, CONFERENCE, "ELECTROCERÁMICA" (CD ROM), 2003, SPAIN, P 91

PHOTOLUMINESCENCE AND QUANTUM YIELDS OF UREA AND URETHANE CROSS-LINKED NANOHYBRIDS DERIVED FROM CARBOXYLIC ACID SOLVOLYSIS

LIANSHE FU, SÁ FERREIRA R A, CARLOS L D, BERMUDEZ DE ZEA V
ORAL COMMUNICATION: EUROPEAN CONGRESS ON ADVANCED MATERIALS AND PROCESSES, LAUSANNE, SUIÇA, 01/09 A 05/09 DE 2003.

PHOTOLUMINESCENT NANOSTRUCTURED FILMS CONTAINING EUROPIUMPOLYOXOTUNGSTATE ANIONS

SOUSA F., FERREIRA A., FERREIRA R., CAVALEIRO A. V., CARLOS L., NOGUEIRA H. I. S., ROCHA J., TRINDADE T.

7TH FIGIPS MEETING IN INORGANIC CHEMISTRY, LISBOA, 2003.

BOOK OF ABSTRACTS, P387

PHOTONICS AND MAGNETISM ON A NANOMETER SCALE OF ORGANIC/INORGANIC HYBRID MATERIALS

CARLOS L D, SÁ FERREIRA R A, SILVA N J O, AMARAL V S, BERMUDEZ DE ZEA V

ORAL COMMUNICATION: II INTERNATIONAL MATERIALS SYMPOSIUM - A MATERIALS SCIENCE FORUM, LISBOA, PORTUGAL (2003)

PLANAR AND UV WRITTEN WAVEGUIDES PREPARED BY ORGANIC-INORGANIC SOL-GEL HYBRIDS BASED ON SILOXANE-POLY(OXYETHYLENE)

MOLINA C, CARLOS L D, GONÇALVES R R, RIBEIRO S J L, MESSADDEQ Y, LEITE A M P P, MARQUES P V S, MOREIRA P J B, BERMUDEZ DE ZEA V, EURONANOFORUM 2003, TRISTE, ITÁLIA (2003)

POLYOXOMETALATES: SYNTHESIS AND APPLICATIONS

CAVALEIRO, A M V

1^{as} JORNADAS DO CICECO

AVEIRO, 19 E 20 DE DEZEMBRO 2003

LIVRO DE RESUMOS, PP 87-88

PREPARATION OF POROUS HYDROXIAPATITE PARTICULES TO BE USED AS DRUG DELIVERY SYSTEMS, M. A. MARTINS, C. SANTOS, M. E. V. COSTA, M. M. ALMEIDA, LIVRO DE RESUMOS DO XI ENCONTRO DA SOCIEDADE PORTUGUESA DE MATERIAIS, MATERIAIS 2003, COSTA DA CAPARICA, 14-16 DE ABRIL DE 2003.

PRODUÇÃO DE EXO-BIOPOLÍMERO POR TRAMETES VERSICOLOR EM DIFERENTES MEIOS DE CULTURA, A.P.M. TAVARES, M.S.M. AGAPITO, J. A. LOPES DA SILVA, A. BARROS, J.A.P. COUTINHO, A.M.R.B. XAVIER, X CONGRESSO NACIONAL DE BIOTECNOLOGIA (LISBON), PORTUGAL, 6-8 DECEMBER 2003.

PRODUCT ENGINEERING VS. PROCESS ENGINEERING ON VOC'S EMISSION.

VILELA, T., PESSOA, P., PEREIRA, P., COUTINHO, J.A.P., KONTOGEORGIS, G.M.,

EUROPEAN CONFERENCE OF CHEMICAL ENGINEERING, GRANADA, ESPANHA, SETEMBRO 2003.

PRODUCTION OF EXO-BIOPOLYMER BY TRAMETES VERSICOLOR UNDER DIFFERENT LIQUID CULTURE MEDIA, A.P.M. TAVARES, J. A. LOPES DA SILVA, A. BARROS, J.A.P. COUTINHO, A.M.R.B. XAVIER, , 11TH EUROPEAN CONGRESS ON BIOTECHNOLOGY, BASEL (SWITZERLAND), AUGUST 2003.

RAMAN AND INFRARED SPECTROSCOPIC STUDIES OF DI-UREASIL NANOHYBRIDS DOPED WITH NEODYMIUM TRIFLATE

CORREIA VILELA I C, BERMUDEZ DE ZEA V, OSTROVSKII D, CARLOS L D 5TH INTERNATIONAL CONFERENCE ON F-ELEMENTS, GENEVA, SUIÇA (2003)

REAPROVEITAMENTO DA LAMA INDUSTRIAL DE MÁRMORE E GRANITO EM MASSAS ARGILOSAS

SILVA J B; ACCHAR W; SEGADÃES A M

RESUMOS DO 47º CONGRESSO BRASILEIRO DE CERÂMICA, JOÃO PESSOA-PB, BRASIL, JUNHO 2003 (REF:5-10).

RECIPROCATING SLIDING WEAR TESTS ON SELF-MATED CVD DIAMOND COATINGS

ABREU C S; BELMONTE M; OLIVEIRA F J; FERNANDES A J S; COSTA F M; SILVA R F; GOMES J R

24TH MEETING OF THE INTERNATIONAL RESEARCH GROUP ON WEAR OF ENGINEERING MATERIALS IRG-OECD, PORTOROZ, SLOVENIA, OCTOBER 16-17, 2003 ("ABSTRACT" AND COMUNICATION)

RELAXORS AT LOW TEMPERATURES: NANODOMAINS OR DIPOLE GLASS, S. VAKHRUSHEV, A. NABEREZHNOV, T. EGAMI, W. DMOWSKI, V.

SHVARTSMAN, A. KHOLKIN, B. DORNER, A. IVANOV

ABSTRACTS OF THE 10TH EUROPEAN MEETING ON FERROELECTRICITY, CAMBRIDGE, UK, 3-8 AUG, 2003, J. OF CONF. ABS. 8. P. 341 (2003).

REMOVING NPE'S FROM KRAFT PULP BLEACHING FILTRATES: ADSORPTION TESTS WITH ZEOLITES AND ACTIVATED

CARBONS. S. SEQUEIRA, A. SILVESTRE, C. PASCOAL NETO, I.

PORTUGAL; COMUNICAÇÃO EM POSTER, 28TH EUCEPA CONFERENCE, LISBOA (2003), P. 338 BOOK OF ABSTRACTS (CD-ROM).

RESEARCH ACTIVITY ON MACROMOLECULAR MATERIALS AND LIGNOCELLULOSICS AT CICECO, C. PASCOAL NETO, A. BARROS TIMMONS, J. COUTINHO, J. CRUZ PINTO, D. EVTUGUIN, I. MARRUCHO, I. PORTUGAL, T. TRINDADE, 1ª JORNADAS DO CICECO, AVEIRO (PORTUGAL), 19-20 DECEMBER.

RESTRICTIONS TO OBTAIN NASICON BY A CERAMIC ROUTE FUENTES R O, LAMAS D G, RAPP M, FIGUEIREDO F M, FRADE J R, MARQUES F M B, FRANCO J I, V CONFERENCIA IBEROAMERICANA EN MATERIALES ELECTROCERÁMICOS, CASTELLÓN, SPAIN, JUNE 19-21, 2003

SAMARIUM AND TERBIUM COMPLEXES OF 2,6-DIHYDROXYBENZOIC ACID

SOARES-SANTOS P. C. R., NOGUEIRA H. I. S., ALMEIDA PAZ F. A., SÁ FERREIRA R. A., CARLOS L. D., KLINOWSKI J., TRINDADE T. 7TH FIGIPS MEETING IN INORGANIC CHEMISTRY, LISBOA, 2003.

SHORT CHAIN DI-UREA CROSS-LINKED HYBRID XEROGELS DOPED WITH ND³⁺ IONS

CORREIA VILELA I C, BERMUDEZ DE ZEA V, CARLOS L D, SÁ FERREIRA R A, ROCHA J, SILVA M M, BARROS S, SMITH M J EUROPEAN CONGRESS ON ADVANCED MATERIALS AND PROCESSES, LAUSANNE, SUIÇA (2003)

SIO₂/ POLY(STYRENE) NANOCOMPOSITES PREPARED BY IN SITU EMULSION POLYMERISATION: SURFACTANTS EFFECT, ESTEVES, A.C.C.; TIMMONS-BARROS, A.M.V.; TRINDADE, T.; LAPCIK, L.J.;, GECE 2003 (GRUPO ESPECIALIZADO EM COLÓIDES E INTERFASES) - COLOIDES E INTERFASES. VIGO (SPAIN), 3-5 JULY 2003.

SOLID STATE ELECTROCHEMISTRY: MATERIALS AND CONCEPTS FOR THE HYDROGEN ECONOMY, REAL FOSSIL FUELS OR ALTERNATIVE FUELS?, FRADE J R, MARQUES F M B, KHARTON V, NAUMOVICH E, FIGUEIREDO F, ABRANTES J, FAGG D P, YAREMCHENKO A, TSIPIS E, SHAULA A, SMIRNOVA O, FERREIRA A A L, HOROVISTIZ A L, 1AS JORNADAS DO CICECO, DEC. 19-20, 2003, AVEIRO, PORTUGAL

SOLID STATE INCLUSION COMPOUND OF S-IBUPROFEN IN β-CYCLODEXTRIN: STRUCTURE AND CHARACTERIZATION BRAGA S S; GONÇALVES I S; HERDTWECK E; TEIXEIRA-DIAS J J C EUROCONFERENCE ON DESIGN AND PREPARATION OF MOLECULAR MATERIALS, ITALY, 2003

SOLUBILITY OF GASES IN PERFLUOROALKANES: EXPERIMENTS AND SAFT MODELING.

DIAS, A.M.A., PÀMIES, J.C., COUTINHO, J.A.P., MARRUCHO, I.M., VEGA, L.F., SAFT '03, ICMAB-CSIC, BARCELONA, ESPANHA, DEZEMBRO 2003.

SOLUBILITY OF OXYGEN IN LIQUID PERFLUOROCARBONS.

DIAS, A.M.A., COUTINHO, J.A.P., MARRUCHO, I.M.,

JORGE CALADO: 40 YEARS OF MOLECULAR THERMODYNAMICS, IST, LISBOA, JANEIRO 2003.

STABILITY AND MIXED CONDUCTIVITY OF NI-CONTAINING PHASES WITH PEROVSKITE- AND K_2NiF_4 -TYPE STRUCTURE

YAREMCHENKO A A; KHARTON V V; SHAULA A L; PATRAKEEV M V; FRADE J R; MARQUES F M B

ABSTRACTS OF THE OSSEP WORKSHOP "IONIC AND MIXED CONDUCTORS: METHODS AND PROCESSES"

2003, AVEIRO, P 44

STRATEGIES FOR THE HETEROGENISATION OF OXOMOLYBDENUM COMPLEXES, M. PILLINGER, C. D. NUNES, S. GAGO, A. S. DIAS, I. S.

GONÇALVES, A. A. VALENTE, T. M. SANTOS, J. ROCHA, 1^{AS} JORNADAS DO CICECO, AVEIRO, 2003.

STRUCTURAL AND DIELECTRIC CHARACTERISTICS OF Ba_2MeWO_6 (Me=Mg, Ni, Zn) DOUBLE PEROVSKITES

KHALYAVIN D D; HAN J; SENOS A M R; MANTAS P Q

BOOK OF ABSTRACTS, XI ENCONTRO SPM

2003, PP5

STRUCTURAL AND DIELECTRIC PROPERTIES OF MG-DOPED STRONTIUM TITANATE CERAMICS: DEPENDENCE ON THE MATERIALS PROCESSING,

A. TKACH, P. M. VILARINHO, A. KHOLKIN, J. PETZELT

ABSTRACTS OF THE 2ND INTERNATIONAL MATERIALS SYMPOSIUM, COSTA DE CAPARICA, 14-16 APR. 2003.

STRUCTURAL AND DIELECTRIC PROPERTIES OF MN-DOPED STRONTIUM TITANATE CERAMICS, A. TKACH, P. M. VILARINHO, A. L. KHOLKIN

ABSTRACTS OF THE 10TH EUROPEAN MEETING ON FERROELECTRICITY, CAMBRIDGE, UK, 3-8 AUG, 2003, J. OF CONF. ABS. 8. P. 331 (2003).

STRUCTURAL AND DYNAMIC STUDY OF THE HYDRATION AND GELATION OF GALACTOMANNAN AND GLUCOMANNAN BY SOLID

STATE ¹³C NMR, M.C. VIEIRA AND A.M.GIL, THE 3RD ALPINE

CONFERENCE ON SOLID-STATE NMR, SETEMBRO 14-18 2003, CHAMONIX-MONT BLANC, FRANCE, (1 PÁGINA).

STRUCTURAL ASPECTS OF OXYGEN IONIC CONDUCTION IN GARNET-, APATITE-, BROWNMILLERITE- AND PEROVSKITE-TYPE FERRITES

VYSHATKO N P; KHARTON V V; MARQUES F M B

ABSTRACTS OF THE OSSEP WORKSHOP "IONIC AND MIXED

CONDUCTORS: METHODS AND PROCESSES", 2003, AVEIRO, P 28

STRUCTURAL CHARACTERISATION OF HETEROXYLANS BY

ELECTROSPRAY TANDEM MASS SPECTROMETRY. REIS, A., PINTO, P.,

COIMBRA, M.A., EVTUGUIN, D.V. , PASCOAL NETO, C., FERRER CORREIA, A.J. AND DOMINGUES, M.R. PROCEEDINGS OF 5TH INTERNATIONAL MEETING OF THE PORTUGUESE CARBOHYDRATE GROUP (GLUPOR 5), SEPT. 7-10. COVILHÃ, P. 34 (2003).

STRUCTURAL PECULIARITIES OF ORGANO-INORGANIC NANOHYBRIDS: VIBRATIONAL SPECTROSCOPIC INVESTIGATION
OSTROVSKII D, BERMUDEZ V. DE ZEA, GONÇALVES M C, JACOBSSON P, CARLOS L D
PRAGUE MEETINGS ON MACROMOLECULES (65TH MEETING - 22ND DISCUSSION CONFERENCE), SPECTROSCOPY OF PARTIALLY ORDERED MACROMOLECULAR SYSTEMS, PRAHA, CZECH REPUBLIC (2003)

STRUCTURAL STUDIES OF KEGGIN-TYPE POLYOXOTUNGSTATES IN DIFFERENT MEDIUM BY EXAFS
BALULA, M S S; SANTOS, I C M S; CAVALEIRO, A M V; SCHLINDWEIN, W
7TH FIGIPS MEETING IN INORGANIC CHEMISTRY
LISBOA, PORTUGAL, 11-14 DE JUNHO, 2003,
BOOK OF ABSTRACTS, P161

STRUCTURE AND DIELECTRIC STUDY OF A LITHIUM NIOBIOSILICATE GLASS SUBMITTED TO A THERMOELECTRIC TREATMENT - M.P.F. GRAÇA, M.A. VALENTE AND M.G. FERREIRA DA SILVA
APRESENTADA NO II INTERNATIONAL MATERIALS SYMPOSIUM REALIZADO NA UNIVERSIDADE NOVA DE LISBOA (CAMPUS DA CAPARICA) EM ABRIL DE 2003.

STRUCTURE OF E. GLOBULUS XYLAN AND ITS BEHAVIOUR DURING PULPING PROCESSES. EVTUGUIN, D.V. , PINTO, P. AND PASCOAL NETO, C. PROCEEDINGS OF 5TH INTERNATIONAL MEETING OF THE PORTUGUESE CARBOHYDRATE GROUP (GLUPOR 5), SEPT. 7-10. COVELHA, P. 27 (2003).
STUDIES ON THE PEROVSKITE-BASED $LA_4SR_{N-4}Ti_NO_{3N+2}$, CANALES-VÁZQUEZ J, TAO S, PATRAKEEV M, IRVINE J T S, ZHOU W, FRADE J R
MATERIALS RESEARCH SOCIETY FALL MEETING, DEC. 1-5, 2003, BOSTON, USA

STUDIES ON THE PEROVSKITE-BASED $LA_4SR_{N-4}Ti_NO_{3N+2}$, CANALES-VÁZQUEZ J, TAO S, PATRAKEEV M, IRVINE J T S, ZHOU W, FRADE J R,
MATERIALS RESEARCH SOCIETY FALL MEETING,
DEC. 1-5, 2003, BOSTON, USA

STUDY OF SINTERING VARIABLES OF TUNGSTEN CARBIDE PARTICLES SPUTTER-DEPOSITED WITH STAINLESS STEEL
FERNANDES C M; SENOS A M R; VIEIRA, M T
BOOK OF ABSTRACTS, XI ENCONTRO SPM, 2003, PP121

SUPRAMOLECULAR COMPLEXES OF CYCLODEXTRINS WITH INORGANIC AND ORGANOMETALLIC GUESTS
RIBEIRO CLARO P J A, ORAL PRESENTATION, PROCEEDINGS OF THE 7TH FIGIPS, LISBON, 11-14 JUNE 2003

SURFACE ORGANOMETALLIC CHEMISTRY: IMMOBILIZATION OF
[SM(OC₆H₂BU^T_{2-2,6-ME-4})₂(THF)₃] AND [SM(OC₆H₂BU^T_{2-2,6-ME-4})₃(THF)] ON
SILICA (500), A. S. DIAS, J. BRANCO, T. A. GASCHÉ, J. CARRETAS, A. A.
VALENTE, J. ROCHA, A. P. MATOS, 7TH FIGIPS MEETING IN INORGANIC
CHEMISTRY, LISBOA, JUNHO, 2003.

SURFACE ORGANOMETALLIC CHEMISTRY: IMMOBILIZATION OF
LANTHANIDE ARYLOXIDES, A. S. DIAS, J. BRANCO, T. A. GASCHÉ, J.
CARRETAS, A. A. VALENTE, J. ROCHA, A. P. MATOS,
7TH FIGIPS MEETING IN INORGANIC CHEMISTRY, LISBOA, JUNHO, 2003.
BOOK OF ABSTRACTS, P. P 216

SYNTHESIS AND CATALYTIC APPLICATIONS OF NEW COMPOUNDS WITH
HETEROPOLYANIONS AND AMINOACIDS
ESTRADA, A C; SANTOS, ICMS; SIMÕES, M M Q; NEVES, M. G. P. M. S;
CAVALEIRO, A M V
7TH FIGIPS MEETING IN INORGANIC CHEMISTRY
LISBOA, PORTUGAL, 11-14 DE JUNHO, 2003
BOOK OF ABSTRACTS, P384

SYNTHESIS AND CHARACTERIZATION OF SRBI₂NB₂O₉ POWDERS
PREPARED BY A NEW CHEMICAL METHOD, GERARDO G. AGUILAR AND
M.ELISABETE V. COSTA, LIVRO DE RESUMOS DO XI ENCONTRO DA
SOCIEDADE PORTUGUESA DE MATERIAIS, MATERIAIS 2003, COSTA DA
CAPARICA, 14-16 DE ABRIL DE 2003.

SYNTHESIS AND CHARACTERISATION OF TWO NOVEL LARGE-PORE
FRAMEWORK VANADIUM SILICATES, P. BRANDÃO, A. A. VALENTE, A.
PHILIPPOU, A. FERREIRA, M. ANDERSON AND J. ROCHA, 26TH ANNUAL
MEETING OF THE BRITISH ZEOLITE ASSOCIATION, NOTTINGHAM, 2003.

SYNTHESIS AND PHOTOLUMINESCENCE FEATURES OF UREA AND
URETHANE CROSS-LINKED SILOXANE-POLY(ETHYLENEOXIDE) HYBRIDS
DERIVED FROM CARBOXYLIC ACID SOLVOLYSIS
LIANSHE FU, CARLOS L D, SÁ FERREIRA R A, BERMUDEZ DE ZEA V
ORAL COMMUNICATION: XI INTERNATIONAL WORKSHOP ON GLASSES,
CERAMICS, HYBRIDS AND NANOCOMPOSITES FROM GELS, SYDNEY,
AUSTRÁLIA (2003)

SYNTHESIS, CHARACTERISATION AND REACTIVITY OF MICROPOROUS
METAL SILICATES, P. BRANDÃO, A. A. VALENTE, J. ROCHA, 1^{AS}
JORNADAS DO CICECO, AVEIRO, 2003.

THE AGEING OF CALCIUM PHOSPHATES IN A SYNTHETIC BLOOD
PLASMA WITH INITIAL PH 7.4, AT 37 °C
INÁCIO P G D, SILVA M C M, CORREIA R N, MAGALHÃES M C F
7TH FIGIPS MEETING IN INORGANIC CHEMISTRY,
UNIVERSIDADE DE LISBOA, PORTUGAL, 11-14 JUNHO 2003
BOOK OF ABSTRACTS P279

THE ALUMINIUM EFFECT ON GEL-DERIVED IRON SILICA GLASSES - M.G. FERREIRA DA SILVA AND M.A. VALENTE
APRESENTADA NA XII INTERNATIONAL WORKSHOP ON SOL-GEL SCIENCE AND TECHNOLOGY REALIZADA EM SYDNEY (AUSTRÁLIA) EM AGOSTO DE 2003.

THE CHEMICAL-PHYSICAL NATURE OF THE WHITE-LIGHT EMISSION FROM AMINE-FUNCTIONALIZED ORGANIC/INORGANIC HYBRIDS
SÁ FERREIRA R A, CARLOS L D, BERMUDEZ DE ZEA V
EUROPEAN CONGRESS ON ADVANCED MATERIALS AND PROCESSES, LAUSANNE, SUIÇA (2003)

THE COMPOSITION OF SOME LIQUID FOODS BY NMR AND LC-NMR/MS, ESSENTIAL TOOL FOR ITS QUALITY CONTROL, I.F. DUARTE, M. GODEJOHANN, U.BRAUMANN, M. SPRAUL AND A.M.GIL, II ENCONTRO LUSO-BRASILEIRO DE RMN, SETEMBRO 23-26 2003, SINTRA, PORTUGAL, (2 PÁGINAS)

THE COMPOSITION OF SOME LIQUID FOODS BY NMR AND LC-NMR/MS, I.F. DUARTE, M. GODEJOHANN, U.BRAUMANN, M. SPRAUL AND A.M.GIL, SMASH 2003, SMALL MOLECULE NMR CONFERENCE, SETEMBRO 14-17, 2003, VERONA, ITÁLIA, (1 PÁGINA)

THE FIRST EXAMPLES OF X-RAY PHOSPHORS, AND C-BAND INFRARED EMITTERS BASED ON MICROPOROUS LANTHANIDE SILICATES
ANANIAS D; RAINHO J; FERREIRA A; CARLOS L D; ROCHA J
5TH INTERNATIONAL CONFERENCE ON F-ELEMENTS ICFE'5, GENEVA, SWITZERLAND, AUGUST 24-29, 2003, P. 128, PC-75.

THE NMR STRUCTURE OF THE C-TERMINAL OF THE PRESEQUENCE OF 5-AMINOLEVOLINATE SYNTHASE (COMUNICAÇÃO EM CARTAZ)
JOSÉ A R FERREIRA, BRIAN J GOODFELLOW, ANJOS L MACEDO, JORGE S DIAZ, GLÓRIA C FERREIRA, PETER HENKLEIN, VICTOR WRAY,
"II ENCONTRO LUSO-BRASILEIRO DE RMN"
SINTRA, PORTUGAL, 23-26 DE SETEMBRO DE 2003

THERMAL TRANSFORMATION OF EU-DOPED MICROPOROUS ZIRCONIUM SILICATE UMBITE STUDIED BY PHOTOLUMINESCENCE
RAINHO J P, ANANIAS D, LIN Z, FERREIRA A, CARLOS L D, ROCHA J
5TH INTERNATIONAL CONFERENCE ON F-ELEMENTS, GENEVA, SUIÇA (2003)

TRANSPORT PROPERTIES OF CGO MODIFIED WITH SINTERING ADDITIVES AND THEIR EFFECTS ON OXYGEN REDUCTION KINETICS
FAGG D P; KHARTON V V; FRADE J R
ABSTRACTS OF THE OSSEP WORKSHOP "IONIC AND MIXED CONDUCTORS: METHODS AND PROCESSES"
2003, AVEIRO, P 22

TRANSPORT PROPERTIES OF LA₂MO₂O₉-BASED MATERIALS

LÓPEZ D M, NUÑEZ P, ABRANTES J C C, FRADE J R
OSSEP WORKSHOP ON IONIC AND MIXED CONDUCTORS: METHODS AND
PROCESSES, AVEIRO, PORTUGAL, APRIL 10-12, 2003

TOXIC EFFECTS OF LEAD CARBONATE ON SPLEEN
TRACANA R B; FERREIRA M E; PEREIRA M L
SETAC EUROPE 13TH ANNUAL MEETING, UNDERSTANDING THE
COMPLEXITY OF ENVIRONMENTAL ISSUES: A WAY TO SUSTAINABILITY,
HAMBURGO, 27 DE ABRIL A 1 DE MAIO DE 2003.

USE OF HIGH FIELD NMR FOR THE STUDY OF BEER, ANA M. GIL, 3RD SYMPOSIUM IN
VINO ANALYTICA SCIENTIA, 10-12 JULHO 2003, AVEIRO. P 15 (1 PÁGINA)

USE OF PERFLUOROCARBONS IN YEAST CULTIVATION.
COELHO, M.A.Z., AMARAL, P.F.F., TAVARES, A.P.M., MARRUCHO, I.M.,
COUTINHO, J.A.P.,
EUROPEAN CONFERENCE OF CHEMICAL ENGINEERING, GRANADA,
ESPANHA, SETEMBRO 2003.

VIBRATIONAL SPECTROSCOPY IN THE STUDY OF MOLECULAR
ASSOCIATION AND SUPRAMOLECULAR STRUCTURES
RIBEIRO-CLARO P J A,
I JORNADAS CICECO, AVEIRO, 19 E 20 DE DEZEMBRO DE 2003

VISCOSITY AND LIQUID DENSITY OF ASYMMETRIC HYDROCARBON
MIXTURES.
QUEIMADA, A.J., MARRUCHO, I.M., COUTINHO, J.A.P., QUIÑONES-
CISNEROS, S.E., STENBY, E.H.
JORGE CALADO: 40 YEARS OF MOLECULAR THERMODYNAMICS, IST,
LISBOA, JANEIRO 2003.

WATER REDUCTION IN ECF KRAFT PULP MILLS: A CASE
STUDY. I. PORTUGAL, T.A. ROCHA-SANTOS, A. DUARTE, C. PASCOAL
NETO; COMUNICAÇÃO EM POSTER, 28TH EUCEPA CONFERENCE, LISBOA
(2003), P. 378 BOOK OF ABSTRACTS (CD-ROM).

ZEOLITES AND ACTIVATED CARBONS FOR THE REMOVAL OF NPE'S
FROM KRAFT PULP BLEACHING FILTRATES. S. SEQUEIRA, A. SILVESTRE,
C. PASCOAL-NETO, I. PORTUGAL; COMUNICAÇÃO EM POSTER, 4TH
EUROPEAN CHEMICAL ENGINEERING CONFERENCE, GRANADA – SPAIN
(2003) P-4.3.048 BOOK OF ABSTRACTS (CD-ROM).

Outras publicações

ALGUMAS RAZÕES PARA UM DEBATE SOBRE FORMAÇÃO DE PROFESSORES ABERTURA DA SEMANA DA PRÁTICA PEDAGÓGICA DA UNIVERSIDADE DE AVEIRO
PEDROSA DE JESUS, JÚLIO, 2003, CIFOP

BIOMINERALIZAÇÃO DE IMPLANTES HUMANOS: SIMULAÇÃO IN VITRO
CORREIA R N; MARQUES P A A P; MAGALHÃES M C F

CATALYTIC OXIDATIVE DELIGNIFICATION WITH KEGGIN-TYPE MOLYBDOPHOSPHATE HETEROPOLYANIONS: APPLICATION TO PULP BLEACHING. PASCOAL NETO, C., COMUNICAÇÃO APRESENTADA PARA CONSÓRCIO DE INDÚSTRIAS DE PASTA CELULÓSICA FINLANDESAS, SEDE DA STORA-ENSO, HELSÍNQUIA, 2003.

CERÂMICOS EM ENGENHARIA BIOMÉDICA - PERSPECTIVA E CASUÍSTICA
CORREIA R N
LIÇÃO-SÍNTESE, PROVAS DE AGREGAÇÃO
2003

COMPOSIÇÃO, ESTRUTURA E COMPORTAMENTO DA MADEIRA DE EUCALYPTUS GLOBULUS NO PROCESSO KRAFT. PASCOAL NETO, C. SEMINÁRIO APRESENTADO NA UNIVERSIDADE FEDERAL DE VIÇOSA, VIÇOSA, BRASIL, 2003.

NANOPARTICLES AND THE ENVIRONMENT , T. TRINDADE, BOOK REVIEW MINERALOGICAL SOCIETY OF AMERICA, 2001, IN CLAY MINERALS, 2003, 38, 255.

PEROVSKITE-RELATED OXIDE MATERIALS FOR OXYGEN-PERMEABLE ELECTROCHEMICAL MEMBRANES
NAUMOVICH E N; YAREMCHENKO A A; VISKUP A P; KHARTON V V
CHEMICAL PROBLEMS OF THE DEVELOPMENT OF NEW MATERIALS AND TECHNOLOGIES
ED: O.A. IVASHKEVICH , BELARUS STATE UNIVERSITY, MINSK, 2003, ISSUE 1, PP 248-263

TÉCNICAS DE AVALIAÇÃO DA FERTILIDADE MASCULINA: APLICAÇÃO A UMA POPULAÇÃO DE RISCO
GOMES A; PEREIRA M L

THE AGEING OF CALCIUM PHOSPHATES IN A SYNTHETIC BLOOD PLASMA WITH INITIAL PH 7.4 AT 37°C
INÁCIO P G D; SILVA M C M; CORREIA R N; MAGALHÃES M C F
7 FIGIPS MEETING, LISBOA, 2003

OUTRAS

ACTIVIDADES

2003

OUTRAS ACTIVIDADES

Organização de Congressos, Workshops e Conferências

Internacionais:

II ENCONTRO LUSO-BRASILEIRO DE RMN, SINTRA, 23-26 SETEMBRO 2003.

OSSEP/ESF WORKSHOP "IONIC AND MIXED CONDUCTORS: METHODS AND PROCESSES", AVEIRO, 10-12 APRIL 2003

16TH CONFERENCE ON CERAMICS IN MEDICINE (BIOCERAMICS 16)
PORTO, NOV 2003

MEMBRO DO COMITÉ INTERNACIONAL DA EUROPEAN EXPERIMENTAL
NMR CONFERENCE, DESDE JUNHO 2002.

Nacionais:

1AS JORNADAS DO CICECO, DEC. 19-20, 2003, UNIVERSIDADE DE AVEIRO,
AVEIRO, PORTUGAL

Organização de Cursos, Seminários e Programas de Formação

CURSO DE FORMAÇÃO ESPECIALIZADA EM BIOMATERIAIS
UNIVERSIDADE DE AVEIRO
2003

SEMINÁRIO: ELEMENTOS INORGÂNICOS NA SAÚDE. TÉCNICAS DE
DIAGNÓSTICO NUMA VISÃO INTERDISCIPLINAR
UA, 25 DE SETEMBRO 2003.

Actividades de Extensão

Ciência Viva, Escolas, etc

ADVANCES IN TECHNOLOGY OF MATERIALS AND MATERIALS PROCESSING JOURNAL (ATM), ISSN 1440-0731
SEGADÃES A M, MEMBRO DO PAINEL DE EDITORES

CIÊNCIA PARA QUÊ? DO CABELO DE BEETHOVEN AO SANGUE ARTIFICIAL

ROCHA J; MARRUCHO I; PEDROSA DE JESUS J D
SEMANA DA CIÊNCIA, CAFÉ DE CIÊNCIA, ESCOLA SECUNDÁRIA DE JOSÉ ESTÊVÃO, AVEIRO, NOVEMBRO 24, 2003

LECTURE ON “NANOCOMPÓSITOS HÍBRIDOS - DA MITOLOGIA À NANOCOMPOSTOS”, CICLO DE CONFERÊNCIAS DO NEQUA (NÚCLEO DE ESTUDANTES DE QUÍMICA DA UNIVERSIDADE DE AVEIRO) IN NOVEMBER 2003.

COMMITTEE OF THE UNIVERSITY OF AVEIRO SCIENCE & TECHNOLOGY WEEK

INTERNATIONAL ADVISORY BOARD OF THE EUROPEAN CONFERENCE ON APPLICATIONS OF POLAR DIELECTRICS

LABORATORY CLASS FOR 11TH YEAR STUDENTS OF CHEMISTRY FROM ESCOLA SECUNDÁRIA JOSÉ ESTEVÃO IN FEBRUARY 2003. THE ACTIVITIES CONSISTED IN THE PREPARATION OF SiO_2 /POLYSTYRENE AND SiO_2 /POLYAMIDE NANOCOMPOSITES.

NANOMATERIAIS: PEQUENAS PEÇAS PARA UM GRANDE PALCO”, SEMANA DA CIÊNCIA E TECNOLOGIA, ESCOLA SECUNDÁRIA DO FUNDÃO, 26 DE NOVEMBRO (2003).

O BINÓMIO DE NEWTON E A VÊNUS DE MILO: UMA QUESTÃO DE PELE 3^{as} JORNADAS SOBRE O ENSINO DAS CIÊNCIAS, ESCOLA SECUNDÁRIA DE TONDELA, MARÇO 2003.

OLIMPIADAS DE QUÍMICA
ORGANIZAÇÃO DA SEMI-FINAL E DA FINAL, AVEIRO, MARÇO E MAIO DE 2003

ORGANIZAÇÃO “CURSO DE PREPARAÇÃO DOS PARTICIPANTES NAS OLIMPIADAS IBERO-AMERICANAS DE QUÍMICA”, AVEIRO, 11,19, 20, 22 E 23 DE SETEMBRO DE 2003

ORIENTAÇÃO DE ESTÁGIOS PEDAGÓGICOS DA LIC. EM ENSINO DE FÍSICA E QUÍMICA

ORGANIZAÇÃO DA SEMANA DA CIÊNCIA E TECNOLOGIA NO DEPARTAMENTO DE ENGENHARIA CERÂMICA E DO VIDRO, SOB O TEMA “DURABILIDADE DOS MATERIAIS”, EM NOVEMBRO DE 2004

PALESTRA DO TIPO “CONVERSA COM OS ALUNOS” DO 8º ANO DE ESCOLARIDADE DA ESCOLA BÁSICA 2,3 DA GAFANHA DA NAZARÉ, INTITULADA A QUÍMICA NO DIA A DIA, 12 E 14 DE MARÇO DE 2003

PIGMENTOS: UM ENCONTRO ENTRE A QUÍMICA E A ARTE”, SEMANA DA CIÊNCIA E TECNOLOGIA, UNIVERSIDADE DE AVEIRO, 28 DE NOVEMBRO (2003)

PROJECTO CIÊNCIA VIVA “EXPERIMENTAR, COMUNICAR E TRANSFORMAR” GERIDO PELO DEPARTAMENTO DE QUÍMICA DA FACULDADE DE CIÊNCIAS DA UNIVERSIDADE DO PORTO

PROCEEDINGS OF “THE SIXTH EUROPEAN CONFERENCE ON APPLICATIONS OF POLAR DIELECTRICS (ECAPD-VI)”
EDITORES: FERREIRA V M; KHOLKIN A; MANTAS P; VILARINHO P; SENOS A M R

SOCIEDADE AMERICANO IEEE-UFFC – MEMBRO DE CONSELHO FERROELÉCTRICO

PROJECTOS

2003

PROJECTOS

31 de Dezembro de 2003

Advanced Electroceramics: Grain Boundary Engineering
COST 525

ALUMINA
(POE- SIME): 00/12.973

Aumento de rendimento de produção de pasta kraft de *Eucalyptus globulus*:
estratégias, mecanismos e impacto na qualidade da pasta
POCTI/EQU/46124/2002

Biolearn- Learning from Nature How to Design Biomimetic Routes for Producing
Calcium-Phosphate Coatings on Polymeric Biomaterials
POCTI/CTM 38803/2001

Boretos Supercondutores: Propriedades e Processamento de Materiais (IR)
POCTI/CTM/39340/2001

Caracterização e reciclagem de lamas derivadas do corte de rochas naturais e ornamentais
Projecto PRAI-Centro

Ceramics and films of incipient ferroelectrics for tunable capacitor applications
SAPIENS 35462/99

Chemical bath deposition of bismuth based pigments
POCTI/QUI/46199/2002

Crescimento de cristais de $\text{SrBi}_2\text{Ta}_2\text{O}_9$ a sua caracterização
F-25.03

Controlling the length scale though chemie douce:from inorganic functional materials
to organic-inorganic hybrids.
POCTI/CTM/46780/2002

Controlo da escala de tamanho através de “Chemie Douce”: de materiais funcionais
inorgânicos a híbridos orgânicos-inorgânicos
POCTI/CTM/46780/2002

CORKPOL- Liquid polyols and polyurethanes from solid agro-forest (cork) residues
POCTI/QUE/33761/2000

Degradation mechanisms in ferroelectric materials via Atomic Force Microscopy
423/DAAD

Deposição de Ceras Parafínicas em Oleodutos
720 B4

Deposição de diamante CVD sobre compósitos cerâmicos nitreto/carboneto de silício
($\text{Si}_3\text{N}_4/\text{SiC}$)
GRICES/CNPq 4.1.3/2001

Descrição de Tensões Interfaciais óleo/água com a Teoria do Gradiente
E-68/03

Desenvolvimento de Condensadores Sintonizáveis para Aplicações nas Frequências
das Micro-ondas
SAPIENS99 35542/99

Desenvolvimento de ferramentas em metal duro revestidas por filmes multicamada
 Si_3N_4 /diamante
Acção Integrada Luso Espanhola Nº E-70/03

Desenvolvimento de formulações, processamento e caracterização de materiais
cerâmicos obtidos a partir de resíduos industriais
GRICES/CAPES (4.1.3/CAPES)

Desenvolvimento de Métodos Experimentais e Teóricos para Caracterização do
Comportamento Tribológico de Materiais Cerâmicos e de Filmes Finos para Aplicações
em Componentes Mecânicos, Especialmente em Selos Mecânicos
GRICES/CAPES Procº. 4.1.3/CAPES

Desenvolvimento de Novos Materiais Microporosos e Mesoporosos Dopados com
Terras Raras para Optoelectrónica
POCTI/32637/CTM/2000

Desenvolvimento Integrado de Processos: produção, separação e purificação de
biopolímeros

Development of a Bioreactor-Based Connective Tissue Production Line (Tissue
Reactor)

CE / G5 RD – CT 2000 – 00282

Development of composites made of cement binders and lignocellulosic materials of
Portuguese origin

POCTI / 1999 / AGR / 35480

Dopagem Electrónica e Propriedades Físicas de Manganitas com Valência Mista

Ecologia industrial: utilização de lamas de ETAR de tratamento de superfície como matéria prima para produção de refractários
POCTI / CTA / 42448 / 2001

Electrical Assisted LFZ Processing for Tailoring Textured Ceramic Materials
POCTI/1999/CTM/35492

Estudo de óxidos com magnetoresistência colossal utilizando isótopos radioactivos no ISOLDE-CERN (IR)
CERN/FNU/49509/2002

Estudo de hidrofluoroéteres como substitutos de CFC's e HFC's'
E-51/02

Estudo do diagrama de fases do C60 a alta pressão e temperatura
POCTI/CTM/40213/2001

Estudos Estruturais por RMN da 5-Aminolevolinato Sintetase (ALAS), a Primeira Enzima do Caminho de Biosíntese do Hemo
POCTI/BME/39184/2001

Estudos de revestimento de suportes de catalizadores cerâmicos (cordierite) e metálicos (aço inóx) com camadas cataliticamente activas
TecnoVeritas

Estudos Estruturais por RMN da 5-Aminolevolinato Sintetase (ALAS), a Primeira Enzima do Caminho de Biosíntese do Hemo
POCTI/BME/39184/2001
Formulação de uma pasta de grés vermelho
Projecto Ceralfa,

Géis com Propriedades Ópticas, Magnéticas e Electroquímicas Inovadoras
POCTI/33653/CTM/2000

Heterogenisation of photochemically and catalytically active transition metal complexes on mesoporous oxides
POCTI/32889/99

Heterogenização de complexos de metais de transição com actividade catalítica
SAPIENS 32889/99

High-Pressure NMR Spectroscopy of Polymers and Biopolymers in CO₂ Emulsions
POCTI/ QUI/ 42313/2001

Immobilization of solvent-stabilized transition metal complexes in micelle-templated silicas and their applications as polymerisation initiators.
Proc AI-A/03 (*Acções Integradas Luso-Alemãs TUM/UA*)

Innovative Gres Porcellanato Tiles Processing
CRAFT, NOVELGRES, Contract No. G1ST-CT-2002-50296,

Integrated process development: production, separation and purification of biopolymers

4.1.3 CAPES

Interactive Calcium-Phosphate Based Materials Prepared by *Post-Hybridization* and *In Situ Hybridization*

POCTI / 1999 / CTM / 35516

Investigação e controlo de barbotinas de enchimento e de moldes com vista à melhoria dos processos de fabrico e da qualidade final dos produtos

Projecto Vista Alegre

Investigation of mechanical and ion transport processes in nickelate-based ceramic membranes under high oxygen chemical potential gradient

INTAS-0276

Lasers em Guias de Onda Ópticos Baseados em Materiais Híbridos Dopados com Iões Lantanídeos Fabricados por Sol-Gel

POCTI/CTM/42478/2001

Ligações de Hidrogénio C-H...O em Líquidos

POCTI/QUI/35408/2000

Materiais Híbridos Orgânicos/Inorgânicos como Matrizes para Compostos

Luminescentes de Iões Lantanídeos

Programa GRICES-CAPES, Cooperação bilateral Portugal-Brasil

Mechanisms of polarization screening and instability in ferroelectric thin films

CZ 4.1.1

Melhoria da brancura das pastas de eucalipto obtidas pelo método do sulfito ácido com base de magnésio

SIME 40/00905/2

Melhoria do rendimento e das características físico-mecânicas das pastas de eucalipto obtidas pelo método do sulfito ácido com base de magnésio

SIME 40/00905/1

Metal/Ceramic Joining for Biomedical Applications: Processing Conditions vs. Microstructure vs. Mechanical and Corrosion

POCTI/1999/CTM/33384

Metodologias de Investigação em Contextos Industriais

3.89.2.5.30

Mixed conducting membranes for partial oxidation of natural gás to synthesis gas

NATO SfP978002

Nanoengenharia de partículas magnéticas e luminescentes para técnicas de separação e marcação de células

3.64.33.7/NANOENGE.../CTS15

Nanomateriais à base de céria para aplicações electroquímicas

Acção integrada Luso-Espanhola No E-49/02

Non-Symmetric macrocycles for metal complexes and supramolecular aggregates with Pesticides

POCTIQUIM/35396/99

Novel Lanthanide Luminescent Systems: from Supramolecular to Nanomaterials

POCTI/QUI/35378/2000

Novos compostos com polioxometalatos e catiões orgânicos: síntese e aplicações catalíticas

POCTI/QUI/38377/2001

Novos compostos com polioxometalatos e moléculas orgânicas dipolares: síntese, caracterização e determinação de propriedades ópticas não lineares

POCTI/CTM/37713/2001

Novos materiais com base em fibras de celulose

3.55.49 (centro de custos)

Optimização da qualidade da superfície de papéis revestidos com pigmentos modificados

POCTI / EQU / 45364 / 2002

Optimização das Propriedades Supercondutoras de Barras Texturadas por Fusão de Zona com Laser Devido à Presença da Fase Bi-2223". Colaborador. Colaboração com a Universidade de Saragoça sob a responsabilidade da Un. Aveiro (Dep. Física).

Acção Integrada Luso Espanhola N° E-50/02

Optimization of paper surface quality with engineered pigments

POCTI/EQU/45364/2002

Permeabilidade de aromas em materiais de embalagem

POCTI/EQU/43356/2001

Permeabilidade de Gases em Matérias de Embalagem

POCTI/43356/EQU/2001

Plasma Simulado para Avaliação In Vitro de Biomateriais

POCTI/QUI/47051/2002

Preparação e caracterização de um novo tipo de membranas baseadas em titanossilicatos

E52/02

Propriedades de transporte e aplicações electroquímicas de nanomateriais à base de céria

POCTI/CTM/39381/2001

Propriedades magnéticas e de transporte de meios nano-granulares bidimensionais e dispositivos sub-micrónicos relacionados
POCTI/CTM/36489/00

QUITOPACK: Development of biodegradable and edible films and coatings based on biopolymers extracted from sea crustacean and mollusc wastes
POCTI/AGR/34804/99

Recycling of Coal Ashes By Glass-Ceramic Technology (Recash)
POCTI/CTM 35482/99

Rede de excelência do papel
UA: 55.50

Rede de Excelência na Área do Papel
PRAI-Centro

Relação entre processamento, estrutura propriedades dieléctricas de cerâmicos à frequência das microondas
POCTI/CTM/40187/2001

Reutilização de Lamas de Estações de Tratamento de Efluentes Industriais
PRAI-Centro

Revestimentos de diamante nanocristalino para aplicações tribológicas em colaboração com o Université Paris 13, Laboratoire d'Ingénierie des Matériaux et des Hautes Pressions, Paris, França.
GRICES/ CNRS Proc. 423/FRANÇA

Simulation of Cyclic Separation using Parallel Computing
POCTI/EQU/46055/2002

Síntese, caracterização estrutural e avaliação do potencial tecnológico de novos materiais de base fosfato
E71/03

Síntese por combustão de cristais alongados de α -Sialon para serem usados como agentes de reforço de CMC processados por via coloidal
POCTI / CTM / 39419 / 2001

Síntese por combustão de nitreto de alumínio (AlN) e processamento de substratos de AlN por tape casting em meio aquoso
Projecto PRAI-Centro

Structural and Functional Aspects of Bulk and Interfacial Polysaccharide-Surfactant Interactions in Food Colloids
33626/99

Structural studies of carbohydrates in the solid state
POCTI/ 33075/QUI/2000

Studies of Colossal Magnetoresistive Oxides with Radioactive Isotopes (IR)
Projecto IS-390 do Laboratório ISOLDE/CERN

Study of pulp and paper industry effluent cleaning by lignolytic cultures of *Trametes versicolor*
POCTI/EQU/48489/2002

Study of the non-covalent adducts of oligodeoxyribonucleotide duplexes with ruthenium(II) complexes by mass spectrometry
SAPIENS 42883/QUI/2001

Study of the viscoelastic properties of Flours: correlation between extensibility and chemical composition
B-9/03

Suportes Compósitos para Engenharia de Tecido Ósseo
CTS2002-05

Synthesis of Chemically Structured Pigments (Kaolin and Calcium Carbonate) for Filler and Coating
POCTI / 1999 / CTM / 36244

Tailored oxomolybdenum catalysts.
POCTI/QUI/37990/2001

Tailored Si₃N₄ –SiC Ceramic Composites for CVD diamond coating”. Director do projecto.
POCTI/1999/CTM/35490

Tailored thin Plasma Polymers for Surface Engineering of Coil Coated Steel

Targeted contrast agents for MRI and nuclear scintigraphy
POCTI/QUI/47005/2002

Técnicas de Diagnóstico Tradicionais e Inovadoras na Biomonitorização da Fertilidade Masculina
CTS/22/2002

Técnicas, ferramentas e paradigmas inovadoras de imagiologia para diagnóstico (colaboração)
CTS/25

Transferência de Energia de Polímeros Electroluminescentes para Dopantes Fosforescentes
POCTI/CTM/40063/2001

Uso de perfluorocarbonetos na aeração de culturas de *Yarrowia lypolitica* para desenvolvimento de bioprocessos e produção de lipase

Valorização de resíduos da fileira floresta para a produção de agregados leves
PRAI Centro – Valorização de resíduos

VEDACERAM – Anéis Vedantes Compósitos de Matriz Cerâmica (Nitreto de Silício) em colaboração com a Durit – Metalurgia Portuguesa do Tungsténio, Lda.
6443 POCTI– Medida 2.3

XAFS studies of hybrid organic-inorganic mesoporous materials
CH1603

XAFS studies of immobilized polymerization catalysts
CH1485

PLANO

DE

ACTIVIDADES

2004

AREA 1

ADVANCED MICRO- AND NANO-STRUCTURE MATERIALS FOR COMMUNICATIONS TECHNOLOGIES

Inorganic Multifunctional Materials and Organic-Inorganic Hybrids

New Microporous Materials. Much work will concentrate on the synthesis and characterisation (structure and photoluminescence, PL) of novel microporous lanthanide silicates. For example, AV-9 materials ($\text{Na}_4\text{K}_2\text{Ln}_2\text{Si}_{16}\text{O}_{38}\cdot 10\text{H}_2\text{O}$, $\text{Ln}=\text{Tb}^{3+}$, Er^{3+}). Work in progress shows that Tb-AV-9 is an efficient X-ray scintillator (using $\text{CuK}\alpha$ radiation). In addition dehydrated Er-AV-9 seems to be an interesting C-band infrared emitter. Microporous zirconium silicate umbite is also being evaluated as a suitable host matrix for hosting Eu(III) ions (in the pores). Upon calcinations, this material yields synthetic (dense) wadeite which seems to be also an interesting PL material. The synthesis, structural characterisation (single-crystal XRD data) and PL properties of novel microporous $[\text{Na}_3(\text{EuSi}_6\text{O}_{15})\cdot 2(\text{H}_2\text{O})]_n$, (AV-21) are under study. The structure of this material seems to be related with that of mineral sazhinite. A considerable amount of research deals with the preparation of films and membranes of microporous materials (luminescent or not). A paper will appear on membranes and films of titanosilicate ETS-10 supported on alumina and stainless steel. Work is in progress to produce such systems doped with lanthanides, exhibiting PL. In an attempt to introduce magnetism into microporous materials, we are working on Cr silicates. The first three-dimensional mixed-metal inorganic-organic hybrid frameworks incorporating N-(phosphonomethyl)iminodiacetate (pmida^{4-}) were prepared and are being characterised by single-crystal XRD. The structures of $[\text{CdVO}(\text{pmida})(4,4'\text{-bpy})(\text{H}_2\text{O})_2]\cdot(4,4'\text{-bpy})_{0.5}\cdot(\text{H}_2\text{O})$ and $[\text{CoVO}(\text{pmida})(4,4'\text{-bpy})(\text{H}_2\text{O})_2]\cdot(4,4'\text{-bpy})_{0.5}$ (where 4,4'-bpy = 4,4'-bipyridine) seem to be identical and are being determined in the $P2_1/c$ monoclinic space group ($Z = 4$).

Mesoporous Materials. Work will continue on functionalise ordered mesoporous silicas with multidentate N-ligands and their use as supports for the heterogenisation of metal complexes with catalytic or photophysical properties. For example, a recently reported method will be used for anchoring of bidentate pyrazolylpyridine L-L ligands on MCM-41. This material will be exposed to complexes of the type $\text{Ln}(\text{NTA})_3$ ($\text{Ln} = \text{Eu}, \text{Gd}$; NTA = naphthoyltrifluoroacetone) with the aim of preparing tethered adducts $\text{Ln}(\text{NTA})_3\text{-L-L}$. In related work, the cyclopentadienyl complex $(\text{RC}_5\text{H}_4)\text{Mo}(\text{CO})_3\text{Cl}$ ($\text{R} = -\text{C}(\text{O})\text{N}(\text{H})-(\text{CH}_2)_3\text{Si}(\text{OEt})_3$) will be prepared and immobilised on MCM-41 by covalent grafting. Subsequently, the material will be treated with *tert*-butyl hydroperoxide (TBHP), in order to convert the tethered complex to a dioxo species of the type $(\text{RC}_5\text{H}_4)\text{MoO}_2\text{Cl}$. CpMoO_2Cl derivatives were recently shown to be active catalysts in the homogeneous liquid-phase epoxidation of olefins using TBHP as oxidant. Our aim is to prepare an equivalent mesoporous heterogeneous catalyst. Work will continue to optimise the synthesis conditions of periodic mesoporous benzene-silica hybrid materials, such as the effect of the type of surfactant template, surfactant/Si ratio, pH, ageing temperature and ageing time. Benzene-silica materials will also be prepared in which a certain fraction of the aromatic groups are functionalised to give $\text{O}_{1.5}\text{Si}-(\eta^6\text{-C}_6\text{H}_4)\text{Cr}(\text{CO})_3\text{-SiO}_{1.5}$ groups. This will be attempted by one-step co-condensation methods or by post-synthesis methods (derivatisation with $\text{Cr}(\text{CO})_3(\text{MeCN})_3$). The local coordination environment of Cr in these materials will be probed by Cr K-edge EXAFS spectroscopy.

Layered Materials. Work is in progress attempting to make layered lanthanide silicates with tuneable photoluminescence. At present we are investigating the synthesis and structural characterisation of the system $\text{K}_3[\text{LnSi}_3\text{O}_8(\text{OH})_2]$, $\text{Ln}=\text{Y}, \text{Eu}, \text{Tb}$ and Er . We are studying layered double hydroxides (LDHs) intercalated with non-steroidal anti-inflammatory drugs and with indomethacin. In the latter case, a pharmacological will also be reported.

The direct synthesis of organometallic-anion-pillared LDHs will be explored, involving the co-precipitation of the component metal hydroxides under controlled pH conditions in the presence of suitable anions, e.g. ferrocenecarboxylate anions. In a different approach, ligands functionalised with carboxylate groups (e.g., 2,2'-bipyridine-5,5'-dicarboxylate) will be introduced into LDHs by ion exchange. These materials will then be studied as "solid ligands" for the immobilisation of different metal complexes ($\text{Mo}^{\text{VI}}, \text{Eu}^{\text{III}}, \text{Gd}^{\text{III}}$). All materials will be characterised by a broad range of techniques, including powder XRD, $^{13}\text{C}/^{27}\text{Al}$ MAS NMR, XAFS spectroscopy, and photoluminescence spectroscopy. The materials containing oxomolybdenum species will also be tested as catalysts for the epoxidation of olefins using TBHP as the oxidant.

LDHs will be prepared and investigated concerning the intercalation possibilities of several types of compounds. Also new Ru(II) complexes with photochemical properties will be used.

Nanostructured Materials. Polyamide-based nanocomposites containing surface-modified SiO₂ nanofillers with different morphologies will be prepared by *in situ* polymerisation. The isothermal crystallisation kinetics will be investigated. Other nanocomposites will be studied, namely polystyrene nanocomposites containing silica-coated Bi₂S₃ nanofibres. The influence of the filler content on the morphology of the nanocomposite particles will be investigated. An anionic surfactant and a reactive monomeric surfactant will be used to obtain nanocomposites with distinct morphological characteristics. Polymer nanocomposites containing CdSe and CdS will be prepared by emulsion polymerisation. The photoluminescence behaviour of such materials will be investigated.

Magnetic nanoparticles of metals and alloys will be prepared using various methods, including reduction of metal salts in aqueous solution and high boiling point solvents. Semiconductor nanoparticles will be synthesised using the single source approach. Functional oxometalates will be prepared. The as-prepared nanoparticles will be investigated as building blocks to fabricate new nanostructures as films and as larger particles.

Novel Pigments. BiVO₄ particles with distinct morphologies will be prepared. The morphosynthesis of these particles will be investigated in detail by SEM and spectroscopic techniques.

Polyoxometallates. Preparation and full structural characterisation of ligands based on lacunary polyoxomolybdates or polyoxotungstates (eg. Keggin-type lacunary tungstophosphate and tungstoborate anions) will be continued. Research will be done on the preparation of coordination compounds of these ligands with both d and f block metals. Ln(III), Fe(III), Ni(II) and Cu(II) ions will be used in the preparation of polyoxometalate complexes and their luminescence and magnetic properties studied. The application of these compounds in the preparation of polyoxometalate-based materials will be explored, namely in the preparation of mono or multilayered nanostructured films and polyoxometalate-anion-pillared layered double hydroxides. Polyoxometalates will be used as inorganic components in the construction of hybrid organic-inorganic functional materials. Film assembly of lanthanopolyoxometalates by electrostatic interactions with organic surfactants will be investigated, together with the formation of new supramolecular polyoxometalate-Ln-organic systems.

New compounds resulting from the association of polyoxometalates organic moieties, in particular chiral aminoacids and aromatic molecules with different substituent groups will be prepared. We shall concentrate on isopolianions like [M₆O₁₉]²⁻ (M = Mo, W, Nb) or [W₁₀O₃₂]⁴⁻, Keggin-type anions like [XM₁₂O₄₀]ⁿ⁻, X=P, Si, B, M = Mo, W and [XW₁₁M'(H₂O)O₃₉]ⁿ⁻, M' = transition ion or other related to these like sandwich-type anions. The compounds are expected to exhibit photochromism or non-linear optical properties or find applications in oxidative catalysis. Following studies on the electrochemical properties of Keggin and sandwich type polyoxometalates, we intend to proceed further with the development of electrodes incorporating these anions and study their possible applications in analysis and electrocatalysis. The incorporation of polyoxoanion salts will be done by adsorption or by multilayer assembly.

Novel Luminescent Systems. Research on novel photoluminescent systems based on lanthanide complexes and its incorporation in nanomaterials will be continued. Research will focus on the coordination chemistry of Ln(III) with derivatised [60]fullerene ligands and aromatic ambidentate ligands, exploring the possibility of formation of multidimensional compounds. The incorporation of such compounds into nanosized SiO₂ and other substrates will be explored considering the possible applications of the resultant materials in optical devices.

A systematic effort will be made to prepare and characterise new complexes of the type Ln(NTA)₃L (Ln = Eu, Gd; NTA = 1-(2-naphthoyl)-3,3,3-trifluoroacetone) containing bidentate N,N-ligands (L = 2,2'-bipyridine, 1,10-phenanthroline and 1,4-diaza-1,3-butadienes). The binuclear complexes (NTA)₃Ln-bpym-Ln(NTA)₃ will also be targets (bpym = 2,2'-bipyrimidine). The photoluminescence properties of these tris-β-diketonate complexes will be of interest because the experimental quantum yield measured for Eu(NTA)₃·2DMSO, 0.75, is one of the highest so far reported for solid state europium complexes.

The photoluminescence features of the remarkable system, Na₃(Y_{1-a}M_a)Si₃O₉ (M=Tb, Tm, Eu), are highly tuneable, depending on the nature and number of different lanthanide ions (up to 3 plus yttrium) in the lattice and on the excitation wavelength. Work in progress suggests that white light and pure red, green and blue colours may be obtained using selected members of the series.

Organic-Inorganic Hybrids Lacking Activating Centres. Work on the discussion of the nature of the emission of white-light photoluminescence sol-gel derived amine-functionalised hybrids lacking metal activator will continue. The focus is on hybrids based on aminopropyltrimethoxysilane, urea (ureapropyltriethoxysilane) or urethane (urethanepropyltriethoxysilane) precursors and classed as aminosils, di-ureasils and di-urethanesils. For the emission ascribed to the siliceous nanodomains the specific photoluminescence mechanism most probably involves silicon-related defects associated with Si-O-Si dangling bonds. The clarification of the nature of those defects-related emitting centers will contribute to the recognition of the paths needed for the development of other efficient photoluminescent siloxane-based hybrids. A new model clarifying the physical mechanisms behind the emission processes will be proposed, considering that the excited carriers can move within localised states, according to the extended multiple trap model. This model will be tested for hydrogenated amorphous silicon and applied to well-known amorphous semiconductors, such as chalcogenide glasses, namely, As_2Se_3 , hydrogenated amorphous carbon alloys of silicon and hydrogen carbon, porous silicon, amorphous silicon carbide and siloxene, $Si_6(OH)_3H_3$, and to the di-ureasil hybrids.

New Hybrid Materials. With the goal of developing innovative hybrid systems with a wide range of useful and tailored properties (e.g. electrochemical, magnetic and optical), class II poly(ethylene)/siloxane composites will be synthesized. In the host framework prepared (*amidossil*) the organic and inorganic counterparts are covalently bonded through amido bridges. The cross-linkages may exist in both sides of the polymer chain or only in one of the terminal sides. The optical and magnetic characterisation of new hybrids based on this hybrid lattice incorporating monovalent (Li^+) divalent (Zn^{2+}) or trivalent (Eu^{3+} and Fe^{3+}) triflate salts will be started.

The magnetic characterisation of bio-inspired iron-doped di-ureasils will continue. The studies will be carried out as a function of the polymer chain length (average number of repeat units 9 - 40), its arrangement and crystallinity, and iron concentration, in order to obtain insight into the self-assembly of magnetic nanoparticles in the hybrid lattice. The synthesis of innovative hybrid hosts with biological components will be attempted. Preliminary work will concentrate on new organic-inorganic hybrids with natural and bio-compatible polymers, such as chitosan and poly(caprolactone). The terminal NH_2 or OH polymer groups will be reacted with the isocyanate group of the siloxane precursor forming new di-ureasils and di-urethanesils.

C60 Phase Transitions Under High Pressure

We are now exploring the top part of the C60 phase diagram ($P > 8 \text{ GPa}$), in particular the phase transformation of C60 into sp^3 superhard phases and polymeric 3D C60 structures. In 2003 new 3D polymeric phases were found. Their structures were not yet determined due to intrinsic disorder and, thus, more experiments are planned for the current year at ESRF-Grenoble.

Development of Spectroscopic Techniques. Work will continue on the development of novel techniques for the study of half-integer quadrupole nuclei in solids, particularly STMAS, FAM and $^{27}Al \rightarrow ^{31}P$ MQ-HETCOR.

The potential of Surface-Enhanced Raman Scattering (SERS) for studying the interaction of metal nanocrystals with molecular adsorbates was explored, in particular in the investigation of adsorption modes and orientation of molecules on the surfaces. Research will now be developed on the use of SERS as a tool for trace detection. Its molecular specificity has potential for resolving a mixture into its individual active components and, thus, it may constitute a method for the detection of, for example, illicit drugs. Several factors will be considered such as: development of new SERS substrates based on metal nanoparticles of Ag, Au and Cu; optimisation of the experimental conditions to obtain good spectra; determination of detection limits for the compounds; study of the selectivity for specific compounds. SERS will also be used to study systems with potential interest in heterogeneous catalysis. Techniques of infrared spectroscopy applied to surface studies will also be explored.

Electroceramics

Microwave Ceramic Dielectrics. Regarding $La(Mg_{1/2}Ti_{1/2})O_3$ (LMT) based microwave dielectric ceramics, a Ph.D. thesis will be defended. Measurements of dielectric characteristics at radio and microwave frequencies will be continued for the LMT based compositions with different substitutions. Work will be carried out on the promising LMT- $BaTiO_3$ and LMT- $SrTiO_3$ systems. Compositions based in solid solutions of LMT and BMW [$Ba(Mg_{1/2}Ti_{1/2})O_3$] will also be evaluated. For the assessment of the major contributing mechanisms far infrared spectroscopy will be used. Structure analysis will continue using techniques such as XRD Rietveld refinements and TEM. The study of the

effect of sintering atmosphere (air, O₂) will be useful to understand the role of certain defects in the dielectric properties.

Solid solutions in the perovskite family allow the change of the temperature coefficient of the permittivity, TC ϵ , of a chosen material. TC ϵ is related with the crystal structure and the crystal status within each structure. The separation of the two possible contributions would greatly improve the knowledge of the phenomenon, thus allowing better materials preparations. This will be explored in the systems Ba₂MgWO₆-Sr₂MgWO₆, where a phase transition between the end members it is expected.

Ferroelectric Ceramics. The work on the morphotropic phase boundary in the PFW-PT system will continue along to major lines: systematic study of the structure and microstructure of the MPB compositions by TEM and HRTEM, from room temperature to 11 K, and evaluation of the piezoelectric and ferroelectric properties of PFW – PT system.

Microstructural design of PZT ceramics will be investigated in order to obtain dense materials with large mean grain size, above 20 μ m. Different methods, such as the use of seeds to favour abnormal grain growth, will be tried. The seeds may be generated locally during sintering or obtained previously by the method of crystal growth (flux growth). Structural and dielectric characterisation of the obtained samples will be initiated.

For high temperature piezoelectric sensor applications, the development of textured ceramics is of fundamental importance to tailor its piezoelectric properties and improve the sensing and actuating performance. SrBi₂Ta₂O₉ textured ceramics will be produced by template grain growth (TGG) using plate-like anisometric SBT single-crystals. Microstructural and electrical characterization will be carried out to evaluate the effects of the ceramic texture degree on its dielectric properties.

Nanoscale Properties of Ferroelectrics. The study of the local properties of ferroelectric thin films and ceramics will be continued. The local properties will be investigated under mechanical stress and electric field. The formation of the nanoscale domains of the size approaching the SFM tip size will be attempted using the effect of mechanical stress-induced domain inversion observed in 2003. The investigations will be extended to a wide range of the compositions and thicknesses of the PZT films of different textures. Piezoelectric ceramics of commercial compositions, piezoelectric composites and multilayer actuators will be investigated at the nanoscale with the aim of improving their electromechanical performance. We plan to extend our activity to antiferroelectric thin films where it may be possible to locally induce a antiferroelectric-ferroelectric phase transition and investigate the nature of the antiferroelectric state at the nanoscale level. We are also planning a new activity dealing with nanolithography and nanopatterning with SFM.

The studies on ferroelectric relaxors will continue, including now new compositions and measurement techniques, in order to gain insight into the nature of the polarization state in relaxors. Pure PMN, freezing at low temperatures, will be investigated using the Peltier cold stage. New materials to be investigated include PMT, SBT:Ce and PFW. Comparison with neutron scattering results will be done, in order to confirm the mean size and distribution of polar clusters obtained by an independent technique. Finally, a new measurement procedure based on nonlinear dielectric spectroscopy will be attempted to visualize the fine polar structure in PMN with higher resolution.

The study of the nature of giant piezoelectric response in PZN-PT single crystals will be extended to the composition PbZn_{1/3}Nb_{2/3}O₃-0.09PbTiO₃, which is closer to the morphotropic phase boundary. The results of the studies on the two compositions will be compared and discussed. The measurements will be complemented with the macroscopic strain observation, aiming at understanding the role of the nanoscale domains in giant piezoelectric response of relaxor single crystals.

The nanoscale study of ferroelectric fatigue in ferroelectric ceramics and thin films will be concentrated on identifying the nature of the defects responsible for fatigue. The nanoscale measurements will be complemented with thermally stimulated currents, conductivity and dielectric impedance spectroscopy. A new physical phenomenon, asymmetric strain hysteresis as a result of fatigue, will be investigated.

Ferroelectric Fibres, Single Crystals and Films. The work conducted until now showed that long sol-gel PZT fibers may be prepared by controlling the acidification of the sol. Long, but cracked, fibres were obtained when methacrylic acid was used. Long polymeric chains were formed in the PZT precursor when C₄H₆O₂ was used and consequently longer fibres were pulled. However, the high amount of organic species that should be released when C₄H₆O₂ is used, definitely contributes to the cracking of the PZT fibers. Based on these results, an organic acid that promotes the formation of long polymeric chains in the precursor, with less content of organics, will be used and studied. Acrylic acid belonging to the same family of methacrylic acid is a good candidate to create long linear polymeric chains in the fibres gel precursors and to improve the macroscopic properties of PZT fibres.

The study of low temperature deposition of ferroelectric films for micromechanical applications will focus on the measurement of the electromechanical properties of the deposited films. The deformation and piezoelectric properties will be investigated as a function of the number of distillations of Pb precursor and the annealing temperature. Voltage piezoelectric coefficients will be evaluated, in order to estimate the suitability of these films as sensors.

BST thin films for potential applications as dielectrics for DRAMs will be prepared by sol – gel. The effect of solvents, such as ethylene glycol and 1,2propanodiol, on the perovskite phase formation, microstructural evolution and dielectric properties will be studied.

In the past years, several scanning force microscopy techniques, including piezoelectric force microscopy (PFM), proved to be powerful for the examination of domain structure, especially on high-ferroelastic distortion systems, because the piezo-coefficient is an important factor affecting the resolution of the domain image. In SBT ceramics and thin films, d_{33} and d_{15} coefficients are several times smaller than in other perovskites. Thus, efforts will address the improvement of the PFM technique, in order to study the domain structure configuration of SBT single crystals.

The method used for the preparation of SBT seeds will be modified to allow the preparation of $\text{SrBi}_2\text{Nb}_2\text{O}_9$ powders. Experimental precipitation conditions will be investigated in view of the close control of the seeds particle size and of the optimisation of the required heat treatments for SBT crystallisation.

SBT seeds produced by the chemical method will be used to improve the synthesis of SBT thin films by a sol-gel procedure, aiming to lower the crystallisation temperature. Characterisation of the unseeded and seeded thin films (XRD, SEM) will be combined with annealing procedures to assess the effects of the seeds on the perovskite phase crystallisation and film microstructure. The investigation of the dielectric and ferroelectric properties of the obtained films will be initiated.

Electrophoretic deposition (EPD) is a simple, rapid and low cost technique to form dense ceramic films with various thickness not obtainable by other techniques. The electrophoretic deposition process will be applied to prepare PZT thick films with thickness in the range 5-200 μm on metal foil. The latter will be used as a substrate for its potential application as embedded capacitors in micro-electronic devices, useful in mobile computing and telecommunications industries. The relation between ageing of suspension, applied dc field, deposition time and film thickness, will be studied. The phase formation process and the reaction layer with the substrate will be optimised by controlling the heat treatment atmosphere. The effect of the sintering conditions on the electrical properties of PZT thick films will be studied.

A photonic sensor equipment will be developed for the electromechanical characterisation of different piezoelectric materials. These studies will be initiated by the electromechanical characterisation of composite, thick and thin films. The film displacement will be studied as a function of the applied field, frequency and temperature. The electromechanical macroscopic response will be compared and related with other electric macroscopic properties and with the local electrical properties measured by SPM.

Incipient Ferroelectrics. The work will continue along two main lines: (i) continuation of the electrical characterisation of Mn doped ST ceramics; the dielectric properties will be measured as a function of temperature and frequency, in a wide frequency range, in order to clearly understand the reasons behind the dielectric relaxation observed in the ST-Mn doped samples; (ii) initiation of the studies on the SrTiO_3 defect chemistry, in order to understand the relationship between the Sr/Ti ratio, microstructure and the dielectric properties.

There is a recent need for SrTiO_3 thin films to be used in microelectronic devices for microwave applications. Due to size and stress effects, it is expected that the structural and dielectric behaviour of incipient ferroelectrics in the thin film and bulk forms are considerably different. The few reported studies are contradictory. A systematic study of doped and undoped ST films prepared by sol-gel will be initiated. The dopants to study are Bi, Mg and Zn. The films will be characterised from the structural, microstructural and dielectric point of view.

Pyrochlores. Novel non-stoichiometric mixed lead and tin niobates with the pyrochlore structure [formula $(\text{Sn}_{1.6-x}\text{Pb}_x)(\text{Nb}_{2-y}\text{Sn}_y)\text{O}_{6.6-0.5y}$, where x (0-1.6) is the Pb(II) and y (0-0.34) is the Sn(IV) contents] have been synthesised via a solid-state route and will be reported soon.

Magnetostructural Modulation of Strongly Correlated Electric (CMR) Materials

Colossal Magnetoresistive Materials. We shall: (i) continue the work on thin film preparation, structural (X-ray), magnetic and electrical properties; study of magnetic and transport properties of CMR manganites and other perovskite derivatives of series R-Ca/Sr-MnO_3 ($\text{R}=\text{La, Pr, Eu, Er, Gd}$) and

Mn substitutions (Cr, Cd); (ii) assemble a RF sputtering deposition system for oxide thin films; (iii) perform a study using implanted radioactive isotopes at ISOLDE-CERN; (iv) carry out a theoretical study of phase transitions and application of non-extensive statistics to manganites; (v) investigate magnetocaloric effects.

High Temperature Superconductors. Physical characterisation studies of oxide superconductor materials prepared by LFZ: magnetic and electrical measurements.

Advanced Molecular and Supramolecular Materials

C-H...O Hydrogen Bonds: Theoretical and Experimental Studies. The importance of C-H...O hydrogen bonds in the molecular association will be assessed for a group of carbonyl-containing systems, using *ab initio* calculations and experimental techniques (vibrational spectroscopy, NMR, Inelastic Neutron Scattering and XRD). Particular attention will be given to the importance of this kind of hydrogen bonding in the formation of supramolecular materials of the so-called “class I” (in which the molecular unities are bound through non-covalent interactions).

Cyclodextrins. The ability of α -cyclodextrin (cyclomalto-heptaose, α CD) to form inclusion complexes has been extensively used in diverse areas such as medicine, catalysis, food chemistry and separation technology. When the guest displays surfactant behaviour, aggregates/micelles of varying dimensions can be formed. The influence of alkali-metal cations and various anions on the inclusion of an amphiphilic guest with surfactant behaviour will continue to be studied.

While many studies on crystalline α CD hydrates have been performed over the years, consideration of the hydration properties of α CD inclusion compounds have not deserved the same attention. Thus, this topic of research will continue.

NMR studies of the α -cyclodextrin/decanoic acid system in the presence of various cations of group 1 halides will be used to determine the conformation of the guest molecule included in various cyclodextrins (α , β and trimethyl). The effect of anions on the α CD–decanoic acid system and on the conformation of the included guest molecule will be studied.

The study of the influence of temperature and co-solvent in inclusion complexes of dimethyl and trimethyl α -cyclodextrins has been motivated by the negative solubility coefficient of both di- and tri-methylated α CDs in water. These cyclodextrins crystallise out of hot aqueous solutions and dissolve in cold water. This research activity aims at assessing the influence of temperature and co-solvents in inclusion complexes of dimethyl and trimethyl derivatives of α -cyclodextrin.

Studies on cyclodextrins as second sphere ligands for metal complexes will continue. Building on previous work, the synthesis and characterisation of inclusion compounds will be expanded to include guests of the type $\text{Ln}(\text{NTA})_3\cdot\text{L}$ (Ln = Eu, Gd; NTA = naphthoyltrifluoroacetone; L = $2\text{H}_2\text{O}$, bipy) and α -CD/ β -CD host molecules. It will be interesting to see how the weak host-guest interaction affects the photoluminescent properties of the guests compared to the non-included complexes. The host-guest interactions will be further explored by carrying out *ab initio* calculations. Another important research area will be the encapsulation of poly(ferrocenylsilanes (e.g., bis-ferrocenylsilane, tris-ferrocenylsilane) within CD host molecules.

Novel Ruthenium Compounds. We shall continue experimental and theoretical studies of a wide range of inorganic and organometallic systems, with a particular focus for complexes containing macrocyclic ligands, namely the study of the interaction host-guest in supramolecular systems involving macrocycles and organic substrates or

metal ions. The results of molecular modelling will be subsequently used in the molecular design of new more efficient receptors in terms of selectivity and binding ability for organic substrates.

The theoretical investigation (molecular mechanics, molecular dynamics and quantum mechanics calculations) of molecular recognition mechanisms involved in the chiral resolution of racemate mixtures by HPLC chiral stationary phases will be carried out. Experimental work will involve single-crystal XRD.

The synthesis and characterisation of novel polypyridyl ruthenium complexes will be continued with a number of new macrocyclic complexes being synthesised via simple substitution reactions and fully characterised by NMR and XRD. Multidentate ligands allowing multinuclear complexes to be constructed will be synthesised and some Ru/Pt complexes prepared. The interaction of complexes with the protein transferrin will be probed by NMR.

The synthesis and characterisation of new Ru(II) complexes with N-aromatic heterocyclic ligands will be carried and tested in redox catalytic applications.

Oxomolybdenum Catalysts. A broad range of complexes of the type $\text{MoO}_2\text{X}_2\text{L}$ were synthesised and tested as catalysts for the epoxidation of olefins, usually employing *tert*-butyl hydroperoxide (TBHP) as the mono-oxygen source. Considerable progress has, therefore, been made in understanding structure-activity relationships, *i.e.* how to obtain active catalysts by appropriate choice of X (Cl, Br, CH_3) and L (Lewis base). Despite these advances, many questions still remain concerning the mechanism of the epoxidation reaction. This will be the focus of future studies. The kinetics of olefin epoxidation in homogeneous phase with $\text{MoO}_2\text{X}_2\text{L}$ -type catalysts and TBHP will be followed by GC-MS, a reaction mechanism proposed and supported by kinetic modelling. These results will be combined with other studies (kinetics of the reaction of $\text{MoO}_2\text{X}_2\text{L}$ with TBHP and DFT calculations) in order to build up a convincing picture of the overall reaction mechanism.

Although good results have been obtained for oxomolybdenum(VI) complexes in homogeneous catalysis, there are drawbacks to consider from an industrial point of view such as the laborious separation of the reagents and products from the catalyst. A promising alternative is to immobilise the catalyst in a room temperature ionic liquid, *i.e.* an organic salt with a melting point below ambient temperature. These novel reaction media are interesting solvents, particularly for catalysis since they are non-volatile, non-flammable, and thermally stable and possess enhanced potential for catalyst separation and recycling. The use of ionic liquids in Mo^{VI} catalyst systems has yet to be investigated. The catalytic performance of dioxomolybdenum(VI) complexes (neutral $\text{MoO}_2\text{Cl}_2\text{L}$ and cationic $[\text{MoO}_2\text{CIL}]\text{BF}_4$) for the epoxidation of olefins with TBHP, using imidazolium-based RTILs as solvents, will be investigated and the results compared with “conventional” one-phase homogeneous catalysis.

Complexes for DNA Probes and Photo and Electrochemical Applications. Compounds displaying DNA-specific binding characteristics and reduced toxicity (for DNA molecular recognition), with transition metal and polypyridyl and/or thioether will continue to be synthesised and characterised. Bridging ligands will be tested to isolate dinuclear systems to evaluate their photo and electrochemical properties.

AREA 2 ADVANCED MATERIALS FOR INDUSTRIAL APPLICATIONS

Reactive Ceramic Components for Process Control

Partial Oxidation of Hydrocarbons and Oxygen Separation. Dense ceramic membranes with mixed oxygen-ionic and electronic conductivity are of great interest for oxygen separation or conversion of methane or natural gas to synthesis gas (syngas). In the near future, we will study the transport properties, surface exchange kinetics and catalytic performance of several mixed conducting materials (e.g. generic compositions $\text{La}_2(\text{Ni}, \text{Co}, \text{Fe})\text{O}_{4+\delta}$ and $\text{La}_{1-x}\text{Sr}_x(\text{Co}, \text{Ga}, \text{Fe})\text{O}_{3-\delta}$), with or without catalysts, porous protective diffusion barriers or other surface modifications. Thermodynamic calculations will be performed to predict the working conditions and requirements (stability and transport properties) of mixed conducting membrane reactors used for partial oxidation of methane combined with water vapour reforming. This study will be extended to account for kinetic limitations. We will try to extract guidelines for the effects of transport properties and surface exchange kinetics of these mixed conductors on methane conversion and selectivity of partial oxidation. *In situ* reduction to form metallic particles (e.g. Ni, Co), other catalysts and composition changes (e.g. use of acidic or basic additives) will be used to assist partial oxidation while avoiding complete oxidation or carbon deposition. Materials which tend to yield complete oxidation will be considered as potential anode components. Microstructural effects will be studied and porous layers will be used to assist the stability of membrane materials and to adjust the kinetics of partial oxidation and/or other surface processes. The catalytic activity of various mixed conductors in the reaction of partial oxidation of methane by atmospheric air will also be studied.

A variety of mixed conductors are being studied as potential membrane materials for oxygen separation or partial oxidation of hydrocarbons. Many of these materials belong to the perovskite-type, which allows a variety of composition changes, such as $(\text{La}, \text{Sr})(\text{Co}, \text{Fe}, \text{Ga}, \text{M})\text{O}_{3-\delta}$, with wide ranges of La and Sr in A sites, Co, Fe, Mg and other additives (Mg, Ga, Ni, Al, ...) in B-sites. $\text{La}_2\text{NiO}_{4+\delta}$ and related layered materials are also being studied in detail. Different routes are being used to prepare these materials, including attempts to obtain textured samples of layered materials in order to optimize the properties. The materials will be characterised in terms of conductivity vs. working conditions, oxygen permeability, surface exchange properties and changes in oxygen stoichiometry. Surface modifications (e.g. additions of a porous layer, metallic or oxide catalysts, etc.) will be used to improve the surface exchange kinetics. The structural and stability issues related to thermal or chemical expansion, chemical stability under reducing conditions, segregation or de-mixing, reactivity with atmospheric gases (e.g. CO_2), etc, will be addressed.

Several composition changes (e.g. $(\text{Sr}, \text{Ca})\text{Fe}_{1-y}\text{Al}_y\text{O}_{3-\delta}$ or $\text{Sr}_{1-x}\text{La}_x\text{Fe}_{1-y}\text{Al}_y\text{O}_{3-\delta}$) are being considered to attain a better compromise between transport properties and stability. Tolerance factor criteria will be used to design new compositions with redox stable additives to obtain enhanced stability and other additives to improve the mixed conductivity of relatively stable materials. These studies include re-examination of ionic and electronic conductivities and their mechanisms, the oxygen stoichiometry, ordering/disordering of point defects and other structural factors affecting ionic motion, thermal or chemical expansion, etc. Titanate-ferrate materials (e.g. $\text{CaTi}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$ and $\text{SrTi}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$) and other materials types will be studied as examples of relatively low cost materials. These will also be used as model materials for structural effects (order/disorder of oxygen vacancies, etc.) on the ionic and mixed conductivity, and to attain a better understanding on how to overcome these limitations.

Two-phase mixed conducting materials will also be studied (e.g. composites containing a ceria based ionic conductor, and a good electronic conductor such as LaMnO_3 or $(\text{La}, \text{Sr})(\text{Co}, \text{Fe})\text{O}_{3-\delta}$). We will attempt to prepare and characterise two-layers membranes by combining materials which meet the requirements of stability and suitable transport properties over different ranges of oxygen chemical potential.

Solid-State Electrochemical Systems and Materials. Envisaged applications will be solid oxide fuel cells, sensors and materials for high temperature electrolysis or oxygen pumping. This requires precise characterisation of electrolyte materials, the corresponding electrodes with thermal and chemical compatibility with the electrolyte and suitable electrocatalytic activity. Laboratory scale devices will be prepared for demonstration and teaching purposes, including a solid oxide fuel cell, an oxygen pump and oxygen sensors of the resistive and potentiometric types. One will attempt to model well-known limitations of potentiometric sensors for minimising these problems and obtaining typical criteria to

assess the validity of sensors readings, taking into account effects of transport properties and their changes with temperature, cell thickness and relevant kinetic parameters.

Electrolytes will be studied with an emphasis on novel materials, relatively inexpensive materials, cationic and protonic conductors. Additives will be used to assist the sinterability and adjust the transport properties. The stability under severe working conditions, undue phase transformations, segregations, etc., of some materials (e.g. $\text{La}_2\text{Mo}_2\text{O}_9$ -based) will be studied in detail, mainly based on refined XRD data, electron microscopy and microanalysis. Addition of Fe to apatite-type materials $\text{La}_{9.83}\text{Si}_{6-x}\text{Al}_x\text{O}_{26+\delta}$ will be used as a model to study relations between composition, structure and properties. XRD and Mössbauer spectroscopy will be used for structural studies, and several techniques will be used to determine transport properties, mainly the modified emf and Faradaic efficiency methods, and the dependence of conductivity and Seebeck coefficient on oxygen partial pressure and temperature.

Layered Na^+ - or K^+ -conducting ceramics such as $\text{Na}_{0.8}(\text{Ni},\text{Ti})\text{O}_2$, $\text{Na}_{0.68}\text{Ni}_{0.34}\text{Ti}_{0.66}\text{O}_2$ and $\text{K}_{0.5+x}(\text{Sb},\text{M})\text{O}_2$, $\text{M}=\text{Mg}, \text{Ni}, \text{Co}$, and NASICON-type materials (e.g. $\text{Na}_3\text{Si}_2\text{Zr}_{1.88}\text{Y}_{0.12}\text{PO}_{11.94}$) will be prepared and characterised by refinement of powder XRD data and electron microscopy. Composition changes will be used to facilitate the sinterability and to improve the stability and/or transport properties. The latter and the applicability of the materials will be studied by total conductivity and emf measurements with water vapour and oxygen concentration cells. Thermal analysis will be used to study the incorporation of water in these materials. A combination of electron microscopy and impedance spectroscopy will be used to study microstructural effects on transport properties. Ageing will also be studied. Some of these cationic conductors will be tested as potentiometric sensor materials.

The development of intermediate-temperature solid oxide fuel cells (IT SOFCs) require novel anode materials with a high electrochemical activity at 800-1070 K. The polarisation of cermet anodes, made of nickel, ceria and yttria-stabilised zirconia (YSZ) and applied onto YSZ solid electrolyte, can be significantly reduced by catalytically-active ceria additions, the relative role of which increases with decreasing temperature. Further improvement is expected by using $\text{Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{2-\delta}$ (CGO), having a high oxygen ionic conductivity, instead of undoped ceria due to enlargement of the electrochemical reaction zone. Nanocrystalline CGO powders will be synthesised via the cellulose-precursor technique and introduced into Ni-CGO-YSZ cermets, and tested in contact with lanthanum based gallate electrolytes.

Sub-micron powders of $\text{La}_2\text{Ni}_{0.8}\text{Cu}_{0.2}\text{O}_{4+\delta}$ with K_2NiF_4 -type structure will also be synthesised via the glycine-nitrate process and used for the preparation of porous cathode layers for lanthanum gallate electrolyte. Cathode layers will be deposited by screen orienting or other suitable methods. We will attempt to demonstrate and understand the effects of transport properties and surface exchange kinetics on the performance of these cathodes.

Composites and Ultra-Hard Coatings for Mechanical Applications

Biomedical Applications of DLC (“Diamond Like Carbon”) and NCD (“Nanocrystalline Diamond”) Coated Si_3N_4 Parts. The underlying idea is to couple Si_3N_4 with an ultra-hard biocompatible film in order to attain outstanding wear and corrosion resistance requirements. Si_3N_4 is a tough ceramic and, if sintered with a proper aid system, a bioactive material. Also, the team’s work in the last years proved the excellent adhesion of CVD diamond to Si_3N_4 substrates. This combination addresses bio applications such as joint implants and medical abrasive tools. Smooth diamond, like NCD, and DLC potentially offers high wear resistance in artificial joints, whereas highly adherent micro-crystalline CVD diamond films on Si_3N_4 for odontologic and orthopaedic burrs anticipates extended lifetime and resistance to sterilisation procedures.

Wear Mechanisms on Hard and Ultra-Hard Materials Machining with CVD Diamond Tools. This work will continue our study of the wear behaviour of new CVD diamond tools produced by CVD thin film (ap. 10 μm) direct coating of Si_3N_4 or by brazing with CVD thick films (>100 μm) onto hard metal (WC-Co) inserts. The grain size of the direct coatings will vary in the range of nanodiamond (< 100nm) to polycrystalline diamond (2-10 μm). These materials will be tested as cutting tools for hard metal, graphite and ceramic materials and their behaviour will be compared with the one of the conventional diamond PCD (“PolyCrystalline Diamond”) and CBN (“cubic boron nitride”) tools. The tool wear behaviour will be investigated in turning operation with assessment of real time forces and contact temperatures and subsequent evaluation of the cutting tip wear by observation in scanning electron and atomic force microscopies, evolution of the cutting edge surface roughness, analysis of the film residual stresses by Raman spectroscopy and evaluation of surface finishing quality of the workpiece by profilometry. The thickness of the CVD diamond, its surface roughness and the geometry of the tool-

cutting tip are parameters that influence cutting forces and thus the wear behaviour of the tools. This study will be carried out in the premises of a collaborating company with a direct interest on the results of the research. Work on CVD diamond coated ceramic materials will continue, the research extending now to the wear of reciprocating couples. An acoustic emission detection system will be used to characterise the fracture/polishing mechanisms of rough diamond and smooth nanodiamond, based on a relationship between the friction coefficient and acoustic emission signals.

Tribological Properties of CVD Diamond. CVD diamond opens the opportunity for applications in machine elements (*e.g.* seals, valves, bearings) and metalworking processes (*e.g.* wire-drawing, extrusion, deep-drawing) that require low friction and high wear resistance. Extremely high hardness and a self-lubricant effect resulting from local graphitisation of diamond in the tribocontact is determinant for this behaviour. To study this, reciprocating sliding ball-on-flat wear tests will be conducted in air, at room temperature, at variable normal load, involving self-mated CVD diamond coated Si_3N_4 couples. Friction and wear results together with characterisation with several techniques (SEM, AFM, micro-Raman) will lead to the comprehension of the tribological response of the system. Ceramic/intermetallic based composites produced by indirect melt infiltration for medium to high temperature mechanical applications will be continued. The ability for these materials to be used as mechanical seals will be evidenced by the study of the wear behaviour of materials with different volume fractions of ceramic and metal under different working conditions (with and without coolant; temperature up to 600 °C). Microstructural and mechanical characterisation of composites will be performed, together with a re-examination of the thermodynamic and kinetic behaviour of these systems.

Other topics will be focussed on the following topics. Coatings of WC and the effect of the coating composition on the thermal reactivity of steel-WC composites in order to eliminate the deleterious ϵ -phase; the mechanical properties of the composites will be also investigated and compared with those of conventional prepared samples. Processing of advanced ceramic and glass-ceramic materials by colloidal shaping techniques using preferentially aqueous media; non-aqueous media will be also used for multicomponent systems that might exhibit some incompatibility in water; new direct shaping methodologies are under development, which will enable de consolidation of large and homogeneous ceramics, including rapid manufacturing. Studies of recycling industrial wastes and by-products to prepare new added-value materials; the current research works will be extended to other residues in order to find solutions to clean the environment, preserve natural and non-renewable resources, save energy, while improving or developing new products. Development of wood-cement composites, *i.e.*, composites made of cement and lignocellulosic materials, namely, forest or agricultural residues, cork residues; besides recycling organic residues, one aims to contribute to better understanding of the effects of extractives from those residues and cement hardening. Precipitated calcium carbonate-based colours for paper coating will be developed using new pigments and processing additives; rheological characterisation of the colours, their coating performance and measurement of the properties of the coating layers and coated papers will be carried out with the aim to establish relationships between the rheology of coatings colours and the properties of the coated layers.

AREA 3

CHEMISTRY AND TECHNOLOGY OF POLYMER AND LIGNOCELLULOSIC MATERIALS AND BIOPOLYMERS

Macromolecular Materials and Lignocellulosics

Lignocellulosics. Research aiming at improving polysaccharides retention and thus improving the pulp yield during *E. globulus* kraft pulping will be pursued. Kraft process modifications, namely (i) the leveling of the sulphide charge along the pulping process, including wood impregnation with sulphide rich liquors and (ii) the addition of borates at different stages of the cooking (including impregnation stage) will be investigated. After this preliminary screening of process modifications, the most promising approach will be selected and the optimisation of process variables will be initiated. The characterisation of the dissolved xylans during the kraft process will be pursued, including the characterisation by sugar analysis, methylation (linkage) analysis, ^1H , ^{13}C and 2D (HSQC, HMBC, TOCSY, NOESY) NMR, ESI-MS and GPC. The studies aiming to assess the influence of kraft process parameters influencing the xylans re-precipitation will be initiated.

The application of Py-GC-MS technique in the fast characterisation of wood and lignins will be continued. The application of the technique in the fast assessment of the global composition of wood will be investigated.

Studies on the surface modification of fibres with alkane-based structures will be pursued. The characterisation of the the previously modified fibres with fatty acids with chain length C6-C22 will be complemented. Composites with such fibres and polypropylene will be prepared and characterised by SEM, TGA, DSC and DMTA. Studies aiming to use vegetable oils and waxes as sources of aliphatic acids for the surface derivatisation of cellulose fibres will be initiated. The preparation of cellulose fibre hybrids with nano-particles will be initiated. Hybrids will be prepared by carrying out the synthesis of inorganic nanoparticles in the presence of cellulose. The nanoparticles to be investigated include TiO_2 , ZnS, ZnO and CaCO_3 , which are white pigments. The conditions of synthesis will be optimised aiming to control the size and shape of particles. Hybrids will be characterised by IR, SEM/TEM, XRD, light scattering and zeta potential measurements. Exploratory blending (under heat application) experiments of selected polymeric matrices and cellulose fibres/inorganic nanoparticles hybrids or modified nanoparticles will be carried out using the most promising systems. Composites will be characterised by SEM/TEM, TGA, DSC and DMTA analysis.

Exploratory experiments aiming to assess wax/cellulose fibres and wax/cork systems as phase change materials for insulation and energy storage applications will be carried out.

The silica-cellulose hybrid materials based on primary sludge and bleached/non-bleached beaten eucalypt kraft pulps will be obtained under optimized conditions in a larger scale. The techniques for the preparation of finish material (molds, etc.) will be developed. Obtained silica-cellulose materials will be tested on water resistance, thermal degradation, thermal conductivity and acoustic properties.

The work on polyoxometalate catalysis in oxygen delignification using combinatory approach with laccase in a multi-stage system for the oxygen bleaching will continue. The efforts will be done to develop the continuous process. A series of polyoxometalates will be deposited on the modified (aminated) cellulose-silica hybrid aiming to use it like support. The new material will be characterised and the possible applications in the oxidation catalysis will be assessed. A series of silica-supported polyoxometalates will be synthesised and tested as oxidative catalysts for the oxidative dehydrogenation synthesis (synthesis of styrene from ethyl benzene).

The investigations on ESI-MS application for the structural characterization of lignin will continue. Using a database obtained from analyses of lignin model compounds, an effort will be done to develop a methodology for the elucidation of lignin oligomers structure from different morphological regions.

The study on the nature of lignin-carbohydrate complexes (LCC) in the eucalypt wood will continue. In order to better understand the NMR data obtained previously on ^{13}C - labeled LCC, a series of LCC model compounds containing phenyl glycoside and benzyl ether type linkages will be synthesised and thoroughly characterised.

The data obtained previously on muconic acid model compound will be extended to the oxidised lignin samples aiming to create a reliable methodology for the detection of muconic acid type structures applying 2D NMR techniques.

A project on the improvement of the yield and the mechanical strength of sulphite pulp will be started. The main idea is to optimise the pulping conditions while the base concentration in the pulping acid increase 1.5-2 times and to estimate the effect of changes made in pulping on the pulp yield, mechanical strength properties and the bleachability.

A project on the improvement of the sulphite pulp brightness in P(O)P bleaching will also be started. The main idea is to optimise the bleaching conditions in order to increase the pulp brightness from actual 89% ISO to 90-91% ISO. The project aims the development of new approaches to reach the stable brightness of 91-92% ISO.

Multidimensional NMR studies for structure determination will be applied to some model compounds of lignocellulosic materials. Site specific ^{13}C labelling will be carried out to aid assignment.

Other Polymer Systems and Materials. Research will continue regarding the preparation of polymer-based nanocomposites via living polymerisation mechanisms such as RAFT and ATRP using mainly emulsion and/or microemulsion techniques. In connection with this work, a collaboration with Carnegie Mellon Univ. is now ongoing. The preparation of nanocomposites based on conducting polymers such as PPY/SiO₂ and their characterisation will continue as they have potential industrial applications as electromagnetic shielding materials.

The characterisation of exo-polysaccharides will be concluded and the preparation and characterisation of nanocomposites will be investigated. The interest in these materials is due to their potential application in packaging, cosmetics and oil recovery.

Studies to improve the flexibility of phenolic resins used in sandpaper production will be carried out in collaboration with a local industry.

In the macromolecular thermal and general dynamic properties, the polymer thermal characterisation and crystallisation studies will now be directed to controlled shear conditions (important in materials processing), and the other studies will focus on refinements of the cooperative segmental theory of molecular dynamics recently developed and its extension to all types of materials' excitation/response, namely creep and stress relaxation.

Continuing to address paraffins as materials and their application, more studies of the crystalline structure of alkylcyclohexanes and alkylbenzenes will be performed. Research on the crystal growth of n-alkanes from complex solutions will also require some attention. Development of composite materials of paraffins with cellulose will be done and its characteristics as insulation and phase change materials will be investigated.

We will try to develop an automated technique to measure vapour-liquid equilibria of polymer solutions, using Head-Space-Gas-Chromatography. Modelling of these systems will be attempted using a molecular based equation of state approach, such as soft-SAFT.

Biomaterials

Biological, Structural and Identification FTIR, NMR and Other Studies. The toxicity effects of new adducts of Cr(V) will continue to be tested in *in vivo* studies with mice, in order to localise and quantify chromium levels in animal organs submitted to severe or chronic intoxication. Histological, histochemical and ultra-structural methods will be the means to characterise the degenerative damage levels caused by those metal complexes and finally to attain occupational purposes. Other techniques such as flow cytometry and fluorescence microscopy will be used to get some more insights into the underlying mechanism of toxicity.

Industrial processes that use transition metal compounds (chromium in its different oxidation states is an example) imply health risks for their workers. Then, the use of fast, reliable and cheap diagnosis techniques for the biomonitoring of their adverse effects is urgent. The application, optimisation and comparison of traditional diagnostic techniques (biopsies) will be compared with new ones (flow cytometry and fluorescence microscopy) in order to evaluate the toxic effects of chromium, cadmium, and lead compounds in male fertility. Mice, previously intoxicated with controlled levels of different metal complexes, will be used as pre-clinical models. The quantification of "dose-effect" relationships is intended, in order to extrapolate for human reproductive risks. Since Aveiro is a highly industrialised region, the establishment of suitable protocols/strategies in the field of occupational health, and the development of a pilot-study in the near future using workers under potential risk, is another purpose of this work.

In vivo studies of chitosan-cardosin as biomaterials will be carried out in collaboration with members of other research units within Aveiro University. The functional aspects of some relevant organs will be tested *in vivo* using mice as models. The chitosan-cardosin association will be applied into mice according to an experimental procedure previously established. The possibility of application of this biomaterial in peritoneal surgery, will be evaluated, specially aiming the prevention of fibrosis. Some biochemical procedures will be used in this evaluation.

Other *in vivo* studies, of the toxicity of some metallic prostheses, will be carried out. The adverse effects of some metallic ions released from some biomaterials used in orthopaedic surgery such as Ti-Al-V and

Cr-Co-Mo based alloys will be investigated in mice using slices of target organs, prepared for histological, histochemical and ultrastructural methods. The possibility of recovery of those effects will be also evaluated. AAS techniques will be used in order to evaluate the content of the metal content within different target organs.

Novel techniques, tools, and paradigms of imagiology for diagnosis will be investigated. A wide range of techniques such as multispectral imaging, life-time imaging, near-infrared imaging, polarisation imaging and Z-scan imaging will be tested in animal cell cultures and tissues, as well as from patients, in order to create a database of high quality images for the diagnosis of some pathologies.

High resolution NMR and MAS NMR will be used, respectively, to monitor biofluids such as bile/urine and kidney tissue samples to investigate possibilities of quick diagnosis of transplant compatibility. LC-NMR/MS and diffusion-ordered spectroscopy (DOSY) will be applied, in tandem with chemometrics, to the quality control of beer and port wine in order to pinpoint origin, process conditions and age; identification of new metabolites with important functional properties will be attempted.

The structure/dynamics of carbohydrate crystals and glasses will be characterised by NMR in tandem with x-ray and other spectroscopic methods. Changes upon glass transition are of particular interest.

The biopolymeric components of flours and their interaction in the whole system will be investigated, as will the dependence on variety and year of harvest. Information will be obtained at both molecular and rheological levels, using a newly developed method to measure extensional deformation.

The NMR study of biomolecules containing paramagnetic metal centres will be continued and applied to some mutants of desulfurodoxin allowing the interactions that stabilise inorganic metal centres in proteins to be probed.

TROSY type experiments will be used to acquire spectra of perdeuterated ^{15}N labelled wild type and mutant 5-Aminolevulinat Synthase (POCTI/BME/39184/2001). The structure of Heme Binding Protein will be determined.

NMR relaxation studies of novel biomedical membranes will be continued. The possibility of applying STM/AFM to these systems, to throw some light on the type of interactions occurring between the polysaccharide and protein that make up the polymer matrix, will be investigated.

Diffusion ordered spectroscopy (DOSY) will be applied to complex mixtures and will be extended to include ligand-substrate systems.

Glass and Ceramic-Based Biomaterials. The processes of crystallisation and ageing of calcium phosphates in SBF solutions with $\text{CO}_2 / \text{HCO}_3^-$ buffer and the analyses of solid calcium phosphates by infrared spectroscopy will be refined.

The influence of several trace metals in the crystallisation and ageing of hydroxyapatite phases will be studied, as well as the crystallisation of magnesium phosphates and their ageing processes in physiological media.

Other topics of research will be the incorporation of larger porous particles in PLGA and PLGA-CaP apatite-coated scaffolds, the transformation of the brushite-chitosan scaffold into hydroxyapatite-chitosan, in addition to drug delivery studies.

Process Development and Optimisation

Phase Behaviour and Transport Properties Relevant in Environmental Protection, Chemical Processing and New Materials Production. On the simulation of cyclic separations using parallel computing, in addition to equipment and numerical library installation, a model of pressure swing adsorption (PSA) will be implemented using sequential and parallel paradigms. A simplified version of SAXS will be re-implemented in C++ (the original code is in C) selecting a general-purpose mathematical model. The model will be used to study a known gas separation case and results compared with available literature. A second sequential version of the model will be introduced in the commercial software gPROMS. This material will constitute the sequential solution or the traditional strategy, which we will use as reference when comparing the parallel solution. While this work is done, the first steps of programming with a parallel scheme will be accomplished. How the problem will be parallelised and an implementation of the code will be established during this period.

A new project will be submitted to FCT, whose objective is the characterisation of new inorganic membranes developed at CICECO. The characterization is achieved: (i) measuring gas permeabilities and selectivities, (ii) carrying out separation of binary gas mixtures, and (iii) studying the influence of temperature upon pure gas permeabilities and gas mixtures separations.

Synthesis of New Materials. Within the biologic reactor studies, after an experimental optimisation of the conditions for production of biopolymer and laccase from *Trametes versicolor*, mathematical modelling of the system will be attempted.

A new FCT project aiming at studying the aeration of biologic reactors starts in 2004. Perfluorocarbons will be used to enhance the oxygen or carbon dioxide availability to the micro-organisms to increase the production of the reactor.

Furfural is made from agricultural raw materials rich in pentosan (polypentose). By aqueous acid catalysis, the pentosan (in particular xylan) is hydrolyzed to pentose, and this pentose is dehydrated to furfural in a unified process. Furfural has a market in the pharmaceutical, agrochemical and polymer fields. Hence, furfural is a key derivative, readily accessible from renewable resources, for the production of a wide range of non-petroleum-derived chemicals. In industrial furfural processes sulfuric acid is used as catalyst, which is extremely corrosive, highly toxic and suffers from drawbacks concerning homogeneous catalytic processes. A possible alternative is to use solid acid catalysts. For example, in 2003 it was reported that the sulfonated resin Amberlyst-15 is an active catalyst for the acid-catalyzed dehydration of fructose. The aim of the present research is to use ordered mesoporous solid acids as catalysts for the liquid-phase dehydration of xylose to furfural. Mesoporous silica functionalised with alkylthiol groups will be prepared either by post-synthesis grafting of purely siliceous MCM-41 or by a one-step co-condensation method. Oxidation of the pendant thiol groups will then give the desired sulfonic acid-functionalised materials. The influence of the physical and chemical properties of the solid acids, reaction time, temperature, solvent, catalyst/xylose ratio on catalytic activity and product selectivity will be studied. Activities will also be compared with homogeneous acid catalysts, such as sulfuric acid and *para*-toluenesulfonic acid.