Session I

João Lopes dos Santos jlsantos@fc.up.pt, (Univ. Porto)
The twisted bilayer: an experimental and theoretical review

A common stacking fault in graphite is a rotation between the layers. This has also been observed directly, both in epitaxial and exfoliated few-layer graphene. A small angle rotation can have profound consequences in electronic properties of the bilayer. I will review some of the experimental observations and theoretical predictions for this curious system.

References

Guohong Li, A. Luican, J. M. B. Lopes dos Santos, A. H. Castro Neto, A. Reina, J. Kong, and E. Y. Andrei.
Observation of van hove singularities in twisted graphene layers. NATURE PHYSICS, advance online publication:
http://dx.doi.org/10.1038/nphys1463 2009.

J. M. B. Lopes dos Santos, N. M. R. Peres, and A. H. Castro Neto.
Graphene bilayer with a twist: Electronic structure. PHYSICAL REVIEW LETTERS, 99(25):256802, DEC 21 2007.

Eduardo Castro evcastro@fc.up.pt, (Instituto de Ciencia de Materiales de Madrid - CSIC, Spain & Centro de Física do Porto)
Acoustic phonon scattering in doped suspended graphene

The two-dimensional allotrope of carbon -- graphene -- has been attracting considerable attention since the first flake was isolated five years ago. The enormous interest is driven equally by the unconventional low-energy behaviour(massless Dirac quasiparticles) and potential technological applications. Recently, suspended graphene samples were shown to have mobilities higher by one order of magnitude than the non-suspended ones. This points to an intrinsic room temperature mobility which is ultimately limited by acoustic phonon scattering. However, recent theoretical approaches taking into account scattering by in-plane acoustic phonons are only partially successful in explaining the experimental data. Here we show that out-of-plane -- flexural -- phonons are even more important and dominate the scattering rate in the relevant temperature region including room temperature. Indeed, taking scattering by acoustic flexural phonons into account provides a better understanding of the experimental data. Based on the flexural phonon sensitivity to whether the graphene membrane is strained or not, we propose a dual gate setup experiment to clearly test the importance of flexural phonons to the scattering rate.

Jaime Santos jaime.santos@fc.up.pt, (Univ. Minho e Univ. Porto)
Electronic doping of graphene by deposited transition metal atoms

In this presentation, we consider the thermodynamic properties of transition metal aggregates (clusters) deposited on graphene, away from full coverage. We present a phenomenological approach that allows us to determine the level of doping of graphene induced by the metal clusters and that also allows us to compute the work function of the joint system. We also consider the contribution of the metal clusters to scattering and to the conductivity of graphene.

Ricardo Mendes Ribeiro ricardo.ribeiro@physics.org, (Univ. Minho)
DFT calculations on graphene

We describe results of density functional calculations of graphene under strain and several types of edge defects on graphene nanoribbons.

Session II

Yuriy Pogorelov ypogorel@fc.up.pt, (Univ. Porto)

Magnetic field strength and orientation effects in CoFe/Al_2 O_3 discontinuous layers close to percolation

H.G. Silva^1,2 , A. M. Pereira^1 , J.M. Teixeira^1 , J. M. Moreira^1 , G. N. Kakazei^1,6 , J. P. Araújo^1 , Yu. G. Pogorelov^1 , J.B. Sousa^1 , M. E. Braga^1, B. Raquet^3 , H. Rakoto^3 , C. Gatel^4 , E. Snoeck^4 , S. Cardoso^5 , and P.P. Freitas^5

/^1 //IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física da Universidade do Porto, Portugal,
^2 //Center of Electronic Optoelectronics and Telecommunications (CEOT), Universidade do Algarve, Campus de Gambelas, 8005-139 Faro, Portugal,
^3 Laboratoire National des Champs Magnétiques Pulsés (LNCMP),
^4 CEMES-CNRS, 29 rue J. Marvig, F-31055 Toulouse Cedex, France ,
^5 / /INESC-MN and IN-Institute of Nanoscience and Nanotechnology, Rua Alves Redol, 9-1, 1000-029 Lisboa, Portugal,/
/^6 //Institute of Magnetism NAS of Ukraine, 36b Vernadskogo Blvd., 03142 Kiev, Ukraine/*//*

Effects of strength and orientation of applied magnetic field in CoFe/Al_2 O_3 –discontinuous layers close to their structural percolation were studied. The study combined the high resolution transmission electronic microscopy (HRTEM) with SQUID magnetometry and ac magnetoresistance measurements. High pulsed magnetic fields up to 35 T were used in the 120 to 310 K temperature range. Comparison was made between longitudinal and transverse(with respect to the film plane) field configurations in the moderate and high-field regimes in order to clarify the nature of the measured negative magnetoresistance. The most important feature of the system is found in the coexistence of two characteristic species of magnetic elements seen from the HRTEM data on CoFe layers: a minority of almost spherical granules of /d/ ~ 3 nm average diameter and a majority of chain-like clusters of such granules of /L/ ~ 20 nm average length, so that the minority mainly controls the tunnel magnetoresistance (TMR) while the majority does the net magnetization. With growing field strength, the temperature dependence of TMR reveals a peculiar inversion, explained by the crossover from Langevin correlations (suppressed with temperature) between magnetic moments in neighbor elements at moderate fields to the correlations in random potential (enhanced with temperature) at high fields. The characteristic field (by minority-majority dipolar coupling) of such crossover ~1 T shows a dimensional enhancement ~ ln(/L///d/) with respect to typical (minority-minority) dipolar field ~ 1 kOe on a granule.

Manuel António Salgueiro da Silva massilva@fc.up.pt, (Univ. Porto)
Electron mass enhancement effects on the spin disorder resistivity of Gd4(Co1-xCux)3 compounds

M A Salgueiro da Silva1,*, T M Seixas1, O F de Lima2, J Lopez2, H F Braun3 and G Eska3
1Departamento de Física da Universidade do Porto, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal
2Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, 13083-970, Campinas, SP, Brazil
3Physikalisches Institut, Universitaet Bayreuth, D - 95440 Bayreuth, Germany

We present a novel combined analysis of the spin disorder resistivity and the electronic specific heat coefficient in Gd4(Co1-xCux)3 compounds, with x = 0.00, 0.05, 0.10, 0.20, 0.30. The experimental results show a strongly non-linear dependence of on the average de Gennes factor (Gav) which, in similar intermetallic compounds, is usually attributed to the existence of spin fluctuations on the Co 3d bands. Values of for these compounds were found around 110 mJ mol-1 K-2, much larger than 38.4 mJ mol-1 K-2 found for the isostructural nonmagnetic Y4Co3 compound. It is shown that the ratio follows a well defined linear dependence on Gav, which is expected when appropriate dependencies with the effective electron mass are taken into account. This indicates that band structure effects, rather than spin fluctuations, could be the main cause for the strong electron scattering and -enhancement observed in the Gd4(Co1-xCux)3 compounds.

Vitor Amaral, vamaral@ua.pt, (Univ. Aveiro)

Nanoscopic scale studies in magnetic and multiferroic materials

V. S. Amaral, Departamento de Física and CICECO, Universidade de Aveiro 3810-193 Aveiro, Portugal

A. L. Kholkin, Departamento de Engenharia Cerâmica e Vidro and CICECO, Universidade de Aveiro 3810-193 Aveiro, Portugal

A. M. L. Lopes, CFNUL, Av. Prof. Gama Pinto 2, 1699 Lisboa, Portugal

J. P. Araújo, Departamento de Física and IN-IFIMUP, Universidade do Porto, 4169-007 Porto, Portugal

P. B. Tavares, Centro de Química-VR, UTAD, 5001-801 Vila Real, Portugal

J. G. Correia, CERN EP, CH 1211 Geneva 23, Switzerland and Instituto Tecnológico Nuclear, E.N. 10, 2686-953 Sacavém, Portugal

Mn^{3+}/Mn^{4} mixed valence manganite systems have very rich phase diagrams exhibiting charge, orbital, magnetic and dielectric competing orders depending on doping, magnetic and electric applied fields, temperature and pressure. The recent interest in multiferroic materials, displaying coexistence of ferroelectricity and magnetic order has triggered further research on these systems. We present studies using the Perturbed Angular Correlations (PAC) technique, with implanted radioactive probes, which allows the determination of Electrical-Field Gradients (EFG) and Hyperfine Magnetic Fields. The reported studies focus on local polaron dynamics, charge orbital mechanisms for multiferroic behaviour and local deformations. Complementary studies of Piezoresponse Force Microscopy (PFM) technique, that uses the detection of local piezoelectric deformation induced by an external electric field at 10 nm level are also reported.

Joao Moreira jmmoreir@fc.up.pt, (Univ. Porto)

New insight on the effect of High Magnetic Field on the metamagnetic Phase Transition of $Gd_5Si_2Ge_2$ and $Tb_5Si_2Ge_2$

A.M. Pereira[1], J.M. Moreira[1], E. Kampert[2] , U. Zeitler[2], C. Magen[3], P.A. Algarabel[4], L. Morellon[3,4], M.R.Ibarra[3,4], J.B. Sousa[1] and J.P. Araújo[1]

[1]*IFIMUP-IN, Physics and Astronomy Department of Science Faculty of Porto University, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal;*
[2] *St Radboud Univ High Field Magnet Lab, 6500 Nijmegen, Netherlands;*
[3] *Instituto de Nanociencia de Aragon Universidade de Zaragoza, 50009 Zaragoza, Spain;*
[4] *Instituto de Ciencia de Aragon Universidade de Zaragoza and Consejo Superior de Investigaciones Cientificas, 50009 Zaragoza, Spain*

Recent scientific and engineering efforts are directed toward s thermomagnetic cooling, since it is considered environmental friendly as it eliminates the use of the traditional chlorofluorocarbons (CFCs) [1]. The $R_5(Si_xGe_{1-x})_4$ alloys are being pointed as the best candidates to be used in thermomagnetic application, due to the large magnetocaloric effect exhibited. Furthermore, these materials exhibit a large magnetoresistivity and colossal magnetostriction [2], which makes then usefulon many other physical applications.

Herein, we present the effect of very high magnetic field (up to 30T) on the magnetization and its ability to induce magnetostructural transition in the paramagnetic phase of $Gd_5Si_2Ge_2$ and $Tb_5Si_2Ge_2$ compounds. We observed that in Gd5Si2Ge2 and $Tb_5Si_2Ge_2$ the competition between the O(I) and M structures arises from the similar free energy between this two structures and concluded that the structural transition is the one responsible for the magnetic state as well as for the first order transitions, whereas the magnetic transition is of pure second order. Based on high magnetic field measurements and using the mean-field theory, we estimated the magnetic temperatures of each structure and concluded that, in the case of the O(I) structure, they are determined by extrapolation of the phase diagram in the Si-rich part.

[1] K.A. Gschneidner Jr. and V.K. Pecharsky, “Thirty years of near room temperature magnetic cooling: Where we are today and future prospects”, International Journal of Refrigeration, vol. 31, no. 6, pp. 945–961, 2008.

A. Gonçalves apg@itn.pt (ITN)

Singularities of U-based intermetallics: the U_2Fe_3Ge case

A.P. Gonçalves[1], M.S. Henriques[1], J.C. Waerenborgh[1], L.C.J. Pereira[1], E.B. Lopes[1], M. Almeida[1], L. Havela[2], O. Tougait[3], H. Noël[3]

[1]Dep. Chemistry, ITN/CFMC-UL, Estrada Nacional 10, P-2686-953 Sacavém, Portugal

[2]Dep. Condensed Matter Physics, Charles University, Ke Karlovu 5, 12116, Prague, Czech Republic

[3]SCR-ECSM/UMR CNRS 6226, Université de Rennes 1, Av. Général Leclerc, 35042 Rennes, France

This talk focuses on the physical properties of U intermetallic compounds, which are directly connected to the particular nature of the 5*f* states. Their energy close to the Fermi level and relatively large spatial extent are responsible for a significant hybridization with the valence states of neighbouring atoms, and hence for their participation in bonding. Moreover, strong spin-orbit interactions frequently exist, which provide a powerful connection between the direction of 5*f* magnetic moments and the crystal structure. This leads to a large diversity in physical behaviors, the nature of the 5*f* electrons being strongly affected by external variables like crystal structure, nature of the nearest-neighbour atoms, magnetic field, temperature, pressure, etc. A main factor that determines the existence of U magnetism is the U-U closest distance ($d_{U\text{-}U}$), the magnetic ordering appearing depending if $d_{U\text{-}U}$ is below or above the Hill limit (~3.4Å) [1].

In this presentation examples of U intermetallics, in particular the U_2Fe_3Ge compound recently studied by us [2] and showing an anomalous exceptional behavior, will be presented and discussed.

U_2Fe_3Ge (Laves C14 structure type) is an intermetallic compound that shows a ferromagnetic like behavior, with a Curie temperature, $T_C = 55$ K, and a spontaneous magnetic moment, $\mu_s = 0.85\ \mu_B$/f.u. The Fe origin of the magnetic ordering can be discarded, as ^{57}Fe Mössbauer spectroscopy exhibits no or very small magnetic hyperfine splittings (the upper limit is ~0.1 μ_B). The very small $d_{U\text{-}U}$ in U_2Fe_3Ge (<2.8Å), well below the Hill limit, made us to perform a thorough study by various experimental techniques. A moderate γ-value, 48 mJ/U-mol K^2, does not step out from the values typical for other U Laves phases, and proves its rather broad band character. The T_C and magnetization decreasing with hydrostatic pressure indicates an itinerant character of magnetism for U_2Fe_3Ge.

References

1. Hill, H.H., Plutonium and Other Actinides 1970, Ed. W.N. Miner, (AIME, New York), 2 (1970).
2. M.S. Henriques, O. Tougait, H. Noel, L.C.J. Pereira, J.C. Waerenborgh, A.P. Gonçalves, Solid State Commun. **148**, 159 (2008).

Session III

Iveta Pimentel iveta@cii.fc.ul.pt, (Univ. Lisboa)

Magnetic Properties of Doped Antiferromagnets

The discovery of superconductivity in the doped copper oxides has stimulated a large number of studies on the magnetism in these materials, both because of its intrinsic interest and its possible connection to high temperature superconductivity. The undoped compounds are antiferromagnetic (AF) insulators, and doping introduces holes, which are the charge carriers, in the spin lattice of the copper oxide planes. The long-range AF order is rapidly destroyed with doping, and superconductivity arises upon further doping, while short-range AF correlations still persist. The CuO2 planes, which are believed to be responsible for the properties of those materials, are described by a spin-1/2 Heisenberg antiferromagnet on a square lattice with moving holes that strongly interact with the spin array. It is therefore important to understand the interplay between spin and charge in those materials.

A striking feature of the copper oxides is the strong dependence of their magnetic properties on the hole concentration. We have studied the effects of doping on a set of magnetic properties, in the framework of t-J model. We have shown that the motion of holes generates significant softening and damping of the spin excitations, and that the long-range AF order, measured by the staggered magnetization, disappears at a small hole concentration due to the decay of spin waves. We have also found that the longitudinal magnetic susceptibility becomes finite in the presence of doping due to the strong damping effects induced by the hole motion, while the transverse magnetic susceptibility is renormalized by softening effects, both susceptibilities increasing with doping, the former more significantly than the latter. In addition, through the calculation of the spin correlation function, we have shown that the motion of holes generates spin fluctuations that add to the quantum fluctuations of the system, and increase with hole concentration. Our results are overall in agreement with experiments on the doped copper oxide superconductors.

Vitalii Dugaev vdugaev@prz.edu.pl, (IST, Rzeszow Univ.)

Spin Hall effect in a two-dimensional electron gas
with a random Rashba spin-orbit interaction

We consider a two-dimensional electron gas in a semiconductor quantum well and several effects related to the spin-orbit coupling. In many cases (for example, in symmetrical quantum wells), the average Rashba spin-orbit interaction is zero but the fluctuations of the Rashba field still exist. Our estimations show that the magnitude of such fluctuations can be large even though it is purely relativistic effect. The main reason is that the electron wavefunction includes a superposition of atomic functions which are localized near the atomic cores.

We considered several different effects related to the fluctuating spin-orbit field. First, we estimated the spin relaxation time of electrons. It gives us an additional mechanism of spin relaxation, which can be comparable to other known effects. We also calculated the combined electron dipole spin resonance and the spin pumping accompanying the absorption of light [1]. In the presented work we will mostly concentrate on a possibility of generation of the spin Hall current. This effect gives us the pure spin current in the 2D electron system with zero average spin-orbit but nonvanishing fluctuations of the Rashba spin-orbit field. Our theory can be also applied to the graphene, where the spatially fluctuating spin-orbit field is related to the ripples at the surface.

V. K. Dugaev, E. Ya. Sherman. V. I. Ivanov, J. Barnas. Phys. Rev. B (Rapid Comm.) **80**, 081301(R) (2009).

M. M. Cruz mmcruz@fc.ul.pt(Univ. Lisboa)
Magnetism in doped wide band semiconductors

M.M.Cruz[1], R.P. Borges[1], C.Silva[1], A.R.G. Costa[1], B. Ribeiro[1] and M.Godinho[1]
[1] *Centro de Física da Matéria Condensada da Universidade de Lisboa / Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal*
R.C. Silva[2,3], L.C. Alves[2,3], N. Franco[2], S. Magalhães[2]
[2] *Laboratório de Feixe de Iões, Dep. Física, Instituto Tecnológico e Nuclear, Estrada Nacional 10, 2686-*
953 Sacavém, Portugal
[3]*Centro de Física Nuclear da Universidade de Lisboa, Av. Prof. Gama Pinto 2,1649-003 Lisboa, Portugal*
The possibility of making devices where spin, rather than charge, controls its function,
integrates the new area of spin electronics, where major developments are being made
in the last years. Diluted magnetic semiconductors (DMS), having magnetic polarized
carriers, are the good materials for bringing together the know-how of traditional
electronics and the spin function, and for that purpose wide band gap semiconductors

doped with magnetic ions have been extensively studied.
In this work, the wide band gap oxides TiO_2 and ZnO doped with the magnetic ions Co,
Ni or Mn, and with non magnetic ions N or Ar were studied.
Single crystals of the oxides were doped using ion implantation at ITN and the implantation profile was followed using Rutherford Backscattering Spectrometry. The
study of the magnetic and electric properties of the obtained systems and its evolution
with annealing treatments was carried out using SQUID magnetometry and magnetotransport measurements, and also Atomic Force Microscopy to follow the
surface morphology.
These studies allowed identifying nano-sized aggregates of the magnetic ions and
characterizing their anisotropy in the case of rutile. These results clearly indicated that
no intrinsic magnetism was observed in these systems. The case of ZnO is different,
aggregation being only detected immediately after implantation in the case of Ni. The
role of defects in the magnetic behaviour of the materials was also addressed with the
study of the samples doped with non magnetic ions. Results indicate a magnetic
contribution of the defects, only stable after thermal treatments in the case of nitrogen
implanted rutile.

David Schmool dschmool@fc.up.pt, (Univ. Porto)

Static and dynamic properties of exchange- spring systems with perpendicular anisotropy

D. S. Schmool[1], N. Sousa[1], A. Apolinario[1], P. Monteiro[1], F. Casoli[2], F. Albertini[2]

[1]*IFIMUP-IN e Departamento de Fisica, Universidade do Porto, Porto, Portugal*

[2]*IMEM – CNR, Parma, Italia*

We have made extensive theoretical and experimental studies in the exchange coupled system consisting of FePt and Fe ferromagnetic layers deposited on MgO substrates. The FePt layer exhibits elevated perpendicular anisotropy and forms in the $L1_0$ ferromagnetic phase. Exchange coupling of such films with an Fe overlayer gives rise to rigid magnet (RM) and exchange spring (ES) systems, depending on the FePt layer thickness. We have performed experimental studies using static magnetic measurements and ferromagnetic resonance (FMR) which can distinguish between these phases. However, a fuller interpretation of the results requires an understanding of the spin configurations in static magnetic fields with

various field strengths and directions. We have performed an extensive study of such static configurations using homemade software and the OOMMF package. Our simulations show the distinct transition from RM to ES states and the further evolution of the ES configuration as a function of the Fe and FePt layer thicknesses. We have also considered the effects of interface conditions, which can have a significant effect on the overall spin configuration. Furthermore dynamic magnetic studies have been made using OOMMF. We will present the results of both experimental and theoretical studies.

Vitor Rocha Vieira vrv@cfif.ist.utl.pt, (IST)
Magnetic dynamics of macrospins in nanosystems

The discovery of the Giant Magnetoresistance in ferromagnetic multi-layers made possible a large increase of the information storage density.
The magnetization dynamics of a nano-scale spin-valve device can be well described by a single magnetic moment (macrospin), which can be studied using the Landau-Lifshitz-Gilbert equation including the Slonczewski spin torque term.
The effect of temperature can be taken into account by the addition of a stochastic magnetic field and a larger device can be studied representing it as a set of interacting macrospins.
In this talk we review the results of the numerical simulations done at CFIF, at IST.

João Amaral jamaral@ua.pt (Univ. Aveiro)
Novel scaling methods for mean-field and critical phenomena analysis of ferromagnetic materials

J. S. Amaral and V. S. Amaral

In this work we explore new methodologies for the analysis of the magnetic properties of ferromagnetic materials. The first scaling method is sustained by the general formulation of the molecular mean-field model, which can encompass magnetoelastic couplings, allowing the study of first-order [1], as well as second-order phase transitions. It is then possible to directly obtain the mean-field exchange parameters from experimental data and the analysis of the scaling function [2]. The second method is based on defining a quantitative goodness of scaling parameter, which allows the search for universal behavior and its respective parameters. We exemplify the use of this method in both mean-field and critical phenomena studies.

We demonstrate the insight obtained from these methods in interpreting phenomena such as magnetic clustering in the ferromagnetic phase in manganite

systems [3], and the study of spin hybridization phenomena in materials with a first-order magneto-structural transition [4,5].

[1] C. P. Bean, and D. S. Rodbell, Phys. Rev. 126, 104 (1962).

[2] J. S. Amaral, N. J. O. Silva, and V. S. Amaral, Appl. Phys. Lett. 91, 172503 (2007).

[3] S. Petit et al., Phys. Rev. Lett. 102, 207201 (2009).

[4] D. Haskel et al., Phys. Rev. Lett. 98, 4 (2007).

[5] L. Pytlik, and A. Zieba, J. Magn. Magn. Mater. 51, 199 (1985).

Session IV

Pedro Alpuim palpuim@fisica.uminho.pt, (Univ. Minho)

Fabrication of thin-film flexible silicon solar cells and other electronic devices

P. Alpuim[1], A. Sammantilleke[1], E. Marins[1], S.Stefanov[2], S.Chiussi[2]

[1] Department of Physics, Universidade do Minho, 4800-058 Guimarães, Portugal

[2] Departamento de Física Aplicada, Universidade de Vigo, 36310 Vigo, Spain

Hydrogenated amorphous silicon (a-Si:H) is a well established technological material that is used at the pixel level in field-effect transistors of flat panel displays to switch on and off the capacitance where the charge controlling the twist of the liquid crystal is stored. Other major applications include solar cells and large-area sensor arrays, like X-ray imaging plates.

All these devices are rigid, since they are fabricated on glass at temperatures in the range 250-350 ºC. In recent years, a new trend for large-area electronic products that are mechanically flexible and will be pervasive in everyday life has been pursued. Thin silicon is a material that can follow this trend, since for thicknesses below ~ 10 µm silicon becomes flexible and bendable to large deflections. However, in case of thin films that are typically less than 500 nm thick the mechanical properties are largely determined by the substrate used. Plastic and stainless steel foils are the most common types of bendable substrates. However, plastics limit the deposition temperature to low values, making it a challenge to keep standard device electronic properties, and stainless steel provides a conductive, rough surface that needs passivation previously to deposition.

In our group a-Si:H solar cells were deposited at a substrate temperature of 150ºC on plastic, in the superstrate p-i-n configuration, and on SiN_x passivated stainless steel in the substrate n-i-p configuration. The efficiency is ~5% in both types of devices, limited by low short-circuit current density and low fill factor. In order to continuously improve the high watt-peak per euro cost ratio, typical of thin film solar cells two directions of research are explored in our work: one is to increase the conversion efficiency of the solar cell by using light trapping effects; the other is to increase the deposition rate of the absorbing layer which translates into a shorter fabrication time that in turn will be reflected in the final cost.

Hydrogenated nanocrystalline silicon (nc-Si:H) is a material parent to a-Si:H that consists of Si nanocrystalls embedded in an a-Si:H matrix. The main advantages when compared to a-Si:H are much higher minority carrier (holes) diffusion length, higher electron and hole mobility and the fact that it does not exhibit Staebler-Wronski effect, responsible for structural and electronic degradation under light exposure in a-Si:H, an important issue in solar cells.

Another important property of doped nc-Si:H films is their piezo-resistivity, i.e. the change in conductivity under strain. We obtained doped nc-Si:H with high negative and positive gauge factors, respectively for n and p-type films, in the range of -30 to 30. Strain sensors based on these films exhibit much higher sensitivity than metallic films and can be miniaturized by using CMOS technology. Piezoresistive strain sensors on polyimide, having mm-size lateral dimensions defined by stencil (shadowing) masks, have been produced and exhibit high linearity and sensitivity.

Using excimer-laser annealing and crystallization (ELA and ELC) we improved crystallinity and dopant activation of very thin (<70 nm) p- and n-type nc-Si:H films deposited on plastic substrates. These highly conductive thin films (σ_{dk} ~ 10-100 $\Omega^{-1}cm^{-1}$) will be used in sensors and, as contact layers, in solar cells.

Carlos Jose Tavares d1916@fisica.uminho.pt, (Univ. Minho)

Enhancement of the photocatalytic nature of nitrogen-doped PVD-grown titanium dioxide thin films on glass and electro-active polymer substrates

Nitrogen-doped titanium dioxide semiconductor photocatalytic thin films have been deposited by unbalanced reactive magnetron sputtering on glass and electroactive PVDF polymer substrates for self-cleaning applications. In order to increase the photocatalytic efficiency of the titania coatings it is important to enhance the catalysts absorption of light from the solar spectra. Bearing this fact in mind, a reduction of the titania semiconductor band-gap has been attempted by using nitrogen doping from a co-reactive gas mixture of N_2:O_2 during the titanium sputtering process. Rutherford Backscattering Spectroscopy was used in order to assess the composition of the titania thin films, whereas Heavy-Ion Elastic Recoil Detection Analysis granted the evaluation of the doping level of nitrogen. X-ray Photoelectron Spectroscopy provided valuable information about the cation-anion binding within the semiconductor lattice. The as-deposited thin films were mostly amorphous, however after a thermal annealing in vacuum at 500 ºC (for those deposited on glass) the crystalline polymorph anatase and rutile phases have been developed, yielding an enhancement of the

crystallinity. Spectroscopic ellipsometry experiments enabled the determination the refractive index of the thin films as a function of the wavelength, whilst from the optical transmittance it was possible to estimate the semiconductor indirect band-gap of these coatings, which has been proven to decrease as the N-doping increases. The photocatalytic performance of the titania films has been characterized by the degradation rate of an organic reactive dye under UV/visible irradiation. It has been found that for a certain critical limit of 1.19 at. % of nitrogen doping in the titania anatase crystalline lattice enhances the photocatalytic behavior of the thin films and it is in accordance with the observed semiconductor band-gap narrowing to 3.18 eV. By doping the titania lattice with nitrogen the photocatalytic activity is enhanced under both UV and visible light.

Keywords：photocatalysis, titania, electroactive polymer, N-doping

Pedro Martins pmartins@fisica.uminho.pt, (Univ. Minho)

Synthesis and characterization of PVDF/CoFe2O4 and PVDF/NiFe2O4 nanocomposites

P. Martins[a], C. M. Costa[b] and S. Lanceros-Mendez[a]*

[a]*Centro de Física da Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal*

[b]CeNTI - Centre for Nanotechnology and Smart Materials, Rua Fernando Mesquita 2785, 4760-034 Vila Nova de Famalicão, Portugal

Multiferroics have invigorated interest in the fields of ferroelectric, ferromagnetic and multifunctional materials as they provide large potential applications in multifunctional devices, transducer, actuators, and sensors. Multiferroic composites are in particular more attractive for studies due to their enhanced properties, particularly at room temperature, in contrast to the single-phase multiferroic materials. Using a solution method, particulate composites films of poly(vinylidene fluoride (PVDF) and $CoFe_2O_4$ and $NiFe_2O_4$ ferrites were prepared.

The nucleation of the beta phase of the polymer was observed in those composites, avoiding the preparation of particulate magnetoelectric composites with stretching at elevated temperature in order to achieve the electroactive β-phase. The differences in the nucleation of the β-phase by the ferrites were detected by Fourier transform infrared spectroscopy and X-ray diffraction. The measured dielectric response demonstrates strong dependence on the weight fraction of ferrite nanoparticles.

ACKNOWLEDGMENTS

We acknowledge the Foundation for Science and Technology (FCT) through the 3º Quadro Comunitario de Apoio, the POCTI and FEDER programs and the PTDC/CTM/69316/2006 and NANO/NMed-SD/0156/2007 projects. P. Martins thanks the support of the FCT (grant SFRH/BD/45265/2008)

Thomas Gasche tpgasche@fc.ul.pt, (Univ. Lisboa)
On the calculation of the cubic and hexagonal phases of BaFeO3

T Gasche1,2 B Ribeiro1 R Borges1 M Godinho1,3

1 CFMC-UL Centro de Física da Matéria Condensada - Universidade de Lisboa, Campo Grande, Ed. C8, 1749-016, Lisboa, Portugal
2 CINAMIL Laboratório de Física, Academia Militar, Lisboa, Portugal
3 Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Campo Grande, Ed. C8, 1749-016, Lisboa, Portugal

BaTiO3 is an architypal ferroelectric where the deviation of the ions from the(high symmetry) cubic structure to a lower symmetry structure gives rise to a electric polarization. The exchange of Fe for Ti could give rise to magnetism and ferroelectric behaviour: a multiferroic.

One of the aims of current experimental work is to stabilize BaFeO3 in a cubic or tetragonal structure, akin to that of BaTiO3. In this paper we report calculations on the bulk hexagonal structure and hypothetical cubic/tetragonal structure in an attempt to identify the differences between them and in order to test the possible role of O vacancies in stabilizing the cubic structure.

Note: This work is part of the simultaneous theoretical/experimental study being carried out on BaFeO3 in the area of multiferroics.

Gonçalo Nuno de Pinho Oliveira goliveira@fc.up.pt, (Univ. Porto)
Local Environment in multiferroic AgCrO2

G. N. Oliveira 1,2, Armandina M. L. Lopes1, Tânia M. Mendonça2, João P. Araújo2, Joaquim A.
Moreira2, Vítor. S. Amaral3, João G. Correia4,5,

1CFNUL, Centro de Física Nuclear, Universidade de Lisboa

2IFIMUP & IN- Instituto de Nanociência e Nanotecnologia, Universidade do Porto

3Departamento de Física e CICECO, Universidade de Aveiro

4ITN, Instituto Tecnológico e Nuclear, Sacavém, Portugal

5CERN – European Organization for Nuclear Research, Genève, Switzerland

The search of new materials with new and/or enhanced physical properties has, nowadays, a strict relation with the evolution of technology. The hunt for systems exhibiting simultaneous (anti)ferroelectric and (anti)ferromagnetic orders has re-started in the last years, and remains as one of the hot topics on Physic and Materials Science scientific communities. This was triggered by the possibility to apply these materials into, e.g., new multiferroic memories that could be written electrically and read magnetically (or vice-versa)[1-3].

Here, we will present an experimental study on one of these so-called multiferroic materials, the $AgCrO_2$ delafossite type compound. The single phase polycrystalline samples of silver chromium oxide $AgCrO_2$, have been prepared by a standard solid state reaction in a O_2 flow. The formation of the $AgCrO_2$ phase was verified through x-ray powder diffraction analysis.

Moreover, magnetic and electric characterization showed that the produced samples have the expected behavior near the ordering temperature (ferroelectric and antiferromagnetic).

In fact, the magnetic susceptibility above TN (21 K) has shown a peculiar behavior, generally attributed to the development of 2D short-range magnetic correlations due to strong frustration coming from antiferromagnetic exchange interactions in a triangular lattice. However, correlating our magnetization results with our Perturbed Angular Correlation data, a slightly different picture emerges. We have evidences that a second local environment emerges below 100 K, possibly due to atomic lattice displacements. Our results suggest that these could be precursor effects of the ferroelectric/antiferromagnetic phase transition.

References:

1. Y.H. Chu, L.W. Martin, et al, Nature Materials 7, 478 (2008).

2. M. Bibes and A. Barthélémy, Nature Materials 7, 425 (2008).

3. S. Seki et al, Phys. Rev. Lett. 101, 067204-1, (2008)

Session V

Manuel Leite de Almeida malmeida@itn.pt (ITN)
1D Systems with conducting and magnetic chains; Magnetic field and pressure effects

Manuel Almeida[a], James S. Brooks[b]

[a] ITN / CFMCUL, EN 10, P-2686-953 Sacavém, Portugal
[b] NHMFL, Florida State University, Tallahassee, FL 32310, USA

The $(Per)_2[M(mnt)_2]$ compounds are an isostructural family containing both conducting stacks of partially oxidized perylene (per) molecules and anionic $[M(mnt)_2]$ stacks, which for some transition metal complexes (M= Ni, Pt, Pd and Fe) may have localized magnetic moments. The two types of chains (conducting and magnetic) in the structure, are both prone to the instabilities typical of conducting and magnetic 1D systems. The low transition temperatures (8-12 K) and the extreme anisotropic electronic band structure make these compounds unique systems to test the behaviour of CDW and magnetic chains under magnetic field. In this communication the recent high magnetic field and pressure studies in these compounds will be summarised

It was found that the CDW state is suppressed at fields of order of the Pauli limit (~23T) with a high conductivity state being recovered. However this suppression presents a significant anisotropy demonstrating non-negligible orbital effects [1]. Furthermore under higher magnetic fields a cascade of new field induced FICDW phases are observed [2]. Hydrostatic pressure in these compounds was found to induce also drastic changes in their ground states. Under moderated pressure there is first a significant reduction of the CDW transition and then, at ≈5 Kbar or above, a metallic state is recovered where the magnetoresistance shows quantum oscillations reaching a quantum limit at circa 20 T. These oscillations are ascribed to Stark interference of electron in open-orbit trajectories

on multiple Fermi surface sheets [3]. The periodicity of the quantum oscillations and angular (AMRO) studies [4] are consistent with a Fermi surface predicted from calculation based on high temperature and ambient pressure structure [5]. More recently in the M=Au compound it was found a superconducting (SC) state at 0.31 K, emerging above 5 kbar in the neighborhood of the CDW [6].

[1] D. Graf, J.S. Brooks, E.S. Choi, S. Uji, J.C. Dias, M. Matos, M. Almeida, *Phys. Rev. B*, **69**, 125113-125117 (2004).
[2] D. Graf, E.S. Choi, J.S. Brooks, R.T. Henriques, M. Almeida, M. Matos, *Phys. Rev. Lett.*, **93,** 076406 (2004).
[3] D. Graf, J.S. Brooks, E.S. Choi, M. Almeida, R. Henriques, J.C. Dias S. Uji, *Phys. Rev. B,* **75**, 245101 (2007).
[4] E. Canadell, M. Almeida, J. Brooks, *Eur. Phys .J. B*, **42**, 453 (2004).
[5] D. Graf, J. S. Brooks, E. S. Choi, M. Almeida, R. T. Henriques, J. C. Dias and S. Uji, *Phys. Rev. B*, **80**, 155104. (2009).
D. Graf, J.S. Brooks, M. Almeida, J.C. Dias, S. Uji, T. Terashima, M. Kimata, *Eur. Phys. Lett.*, **85**, 27009 (2009).

Jose Carmelo carmelo@fisica.uminho.pt (Univ. Minho)

d-wave superconductivity in a square-lattice quantum liquid perturbed by weak 3D uniaxial anisotropy

d-wave superconductivity in a square-lattice quantum liquid perturbed by weak 3D uniaxial anisotropy.
We consider the quantum system obtained from perturbing the square-lattice quantum liquid introduced in Ref. [1] by weak three-dimensional (3D) uniaxial anisotropy. We present preliminary results on the relation of our theoretical scheme to the unusual physics of five representative hole-doped cuprate superconductors with lower and upper dome critical hole concentrations 0.05 and 0.27, respectively. That analysis seems to indicate that combining the electronic correlations described by the square-lattice quantum liquid perturbed by 3D uniaxial anisotropy with the very weak effects of intrinsic disorder or superfluid-density anisotropy leads for the hole-concentration range (0.05,0.27) to a successful description of the universal properties of the representative systems.

[1] - J. M. P. Carmelo, The square-lattice quantum liquid of charge c fermions and spin-neutral two-spinon s1 fermions. Nuclear Physics B 824, 452-538 (2010).

Antonio Miguel Garcia-Garcia <agarcia@cfif.ist.utl.pt> , (IST)

Finite size effects in BCS superconductivity: theory and experiments

We combine the BCS self-consistency condition, a semiclassical expansion for the spectral density and interaction matrix elements to describe analytically how the superconducting gap and the critical temperature depend on the size and shape of a 2d and 3d superconducting grain. Measurements by scanning tunneling spectroscopy on single isolated

Sn nanoparticles confirm the theoretical predictions. Based on these results we discuss different possibilities to increase the critical temperature of a superconductor.

Luis Miguel Fortuna Rodrigues Martelo martelo@fe.up.pt (Univ. Porto)
Exact solution for a boson-fermion model and application to ultra-cold atoms

L. M. Martelo (1) and N. Andrei (2)

(1) *Physics Eng. Dept., Faculty of Engineering, University of Porto,*

P-4200-465 Porto, Portugal and CFP, Faculty of Sciences, University of Porto, P-4169-007 Porto, Portugal

(2) *Physics and Astronomy Dept., Rutgers University,Piscataway, New Jersey, NJ 08854, USA*

The progress on ultra-cold atoms experiments allowing to tune fermionic systems through a Freshbach resonance where itinerant fermionic atoms may form tightly bound pairs ("bosonic" molecules) [M.W. Zwierlein et al., "Observation of Bose-Einstein Condensation of Molecules", Phys. Rev. Lett. 91, 250401 (2003); C. A. Regal et al.,"Observation of Resonance Condensation of Fermionic Atom Pairs", Phys. Rev. Lett. 92, 040403 (2004)] has lead to a renewed theoretical interest in boson-fermion models. We study a 1D boson fermion resonance model describing itinerant spin-1/2 fermions and itinerant scalar bosons coupled through a local interaction which describes the binding of a pair of opposite spin fermions to form a scalar boson, and the reverse process. The model also includes a detuning term characterized by a detuning parameter.
It is found that the model has an exact solution by Bethe Ansatz . We find that the model supports fermion bound pairs. For sufficiently large values of the detuning parameter the ground state consists of purely unbound fermions forming a Fermi liquid. As one decreases the detuning parameter the system goes through a Feshbach resonance and the ground state becomes unstable with respect to the formation of bound fermion

pairs. In this case unbound fermions and bound fermions pairs coexist. The BCS-BEC scenario will also be discussed.

Patrizia Monachesi patrizia.monachesi@aquila.infn.it, (Univ. dell'Aquila e Univ. Lisboa)
Metallic Surfaces as Optical Probes for Absorption of Organic Molecules

The surfaces of noble metals and aluminum are substrates for the preparation of organo-metallic devices with application in bio-electronics. The interface properties depend on both the molecule and the substrate and can be studied by optical spectroscopy with different techniques. We show that electronic calculations made within Density Functional Theory in Local Density Approximation can provide either the spectra to be compared directly with the experimental ones or allow one to obtain 'ab initio' quantities, like Densities of States, Adsorption Energy and geometrical factors of the adsorbate. Results for different systems/techniques will be presented. Reflectance Anisotropy Spectra are the fingerprint of the surface as shown for CO/Cu(110) [1] from the clean to the saturation coverage. High Resolution Photoemission, in combination with Density of States calculation of the interface, is able to highlight the properties of the surface as well as those of the molecule head-group, as for mercapto-benzo-xazole, a thiol, on Cu(001) [2,3]. Finally, Electron Energy Loss Spectroscopy is adequate to analyze the interface among aromatic rings on Al surface, where they form weak bonding, as shown by the pyrrole molecule on [4] Al(001).

References:

1. Optical Response of Copper Surface to Carbon Monoxide Deposition
P. Monachesi and L. Chiodo, Phys. Rev. Lett. 93, 116102 (2004)
2. Anchoring of sulfur-headgroup organic molecules at Cu (100): tayloring the interface electronic states
M.G Betti, F Bussolotti, L. Chiodo, P. Monachesi, C. Mariani, Surf. Scie. 601, 2580 (2007)
3. Role of coverage an the electron properties of sulfur chemisorbed on Cu(100): ab initio calculations, L. Chiodo and P. Monachesi, Phys.Rev.R B75, 075404 (2007)
4. Experimental and Theoretical Investigation of the Pyrrole/Al(100) Interface,
A. Ruocco, L. Chiodo, M. Sforzini, M. Palummo, P. Monachesi and G.Stefani J. Phys. Chem. A, Article ASAP (DOI: 10.1021/jp905537g),October 29, (2009)

Session VI

Joao Luis Maia Figueirinhas figuei@cii.fc.ul.pt, (IST)

Molecular order studies in V shaped mesogens exhibiting a biaxial nematic phase using Deuterium NMR

João L. Figueirinhas[a,b], Carlos Cruz[a,b], Gabriel Feio[c], Matthias Lehmann[d], Christiane Köhn[d]

a IST, Dep. de Física, Av. Rovisco Pais, P-1049-001 Lisboa, Portugal

b CFMC, Av. Prof. Gama Pinto, 2, P-1649-003 Lisboa, Portugal

c CENIMAT/I3N, FCT-UNL, , P-2829-516 Caparica, Portugal

d Chemnitz University of Technology, Institute of Chemistry, Non-Classical Synthetic Methods, Straße der Nationen 62, 09111 Chemnitz, Germany

The biaxial nematic phase was theoretically predicted by Freiser in 1970[1] but was only undoubtedly identified by several independent experimental techniques[2], in low-molecular weight thermotropic liquid crystals, in 2004. The recent synthesis of a new series of shape persistent V-shaped mesogens with four lateral aliphatic chains and different types of bending units opened new trends of phase engineering in the search for stable biaxial nematic phases[3]. Deuterium NMR spectroscopy is one of the leading techniques to investigate biaxial ordering[4]. Optical studies and X-Ray diffraction measurements on aligned samples have produced compelling evidence for the presence of biaxial nematic ordering in

nematogens with fluorenone bending units exhibiting monotropic nematic domains[5]. These results are supported by the deuterium NMR measurements reported in in this work, performed in a deuterated derivative of the V-shaped compounds. The analysis of the deuterium NMR spectra clearly shows the presence of biaxial ordering in the nematic glass.

(1) M. J. Freiser, *Phys. Rev. Lett.* **1970**, *24*, 1041 (1970)

(2) L. A. Madsen, T. J. Dingemans, M. Nakata and E. T. Samulski, *Phys. Rev. Lett*. **2004**, *92*, 145505; B.R. Acharya, A. Primak, and S. Kumar, *Phys. Rev. Lett*. **2004**, *92*, 145506

(3) M. Lehmann, C. Köhn, H. Kresse and Z. Vakhovskaya, *Chem. Comm*. **2008**, 1768

(4) G. R. Luckhurst, *Thin Solid Films* **2001,** *393*, 40

(5) M. Lehmann,S.-W. Kang, C. Köhn, S. Haseloh, U. Kolb, D. Schollmeyer, Q. Wang and S. Kumar, *J. Mater. Chem*. **2006***, 16*, 4326

Carlos Manuel dos Santos Rodrigues da Cruz carlos.cruz@ist.utl.pt (IST)

Molecular structure and biaxial nematic ordering in thermotropic liquid crystals

C. Cruz[1,2], J.L. Figueirinhas[1,2], P.J. Sebastião[1,2], M. Cardoso[2], D. Filip[2], A.C. Ribeiro[1,2], G. Feio[3], M. Vilfan[4], D. Apreutesei[5], T. Meyer[5], P.H.J. Kouwer[5] and G. H. Mehl[5]

[1] Dep. Física, Instituto Superior Técnico, TU-Lisbon, Avenida Rovisco Pais P-1040-001 Lisboa, Portugal
[2] CFMC, Universidade de Lisboa, Av. Prof. Gama Pinto 2, P-1649-003 Lisboa, Portugal
[3] CENIMAT, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal[4] Jozef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

[5] **Department of Chemistry, University of Hull, Cottingham Rd, Hull, HU6 7RX, United Kingdom**

The search of thermotropic liquid crystals exhibiting the biaxial nematic phase has been an active field of investigation since the theoretical prediction of this mesophase by Fraiser in 1970 [1, 2, 3]. The initial synthetic trend in the search of this type of materials was mainly directed to the creation of mesogenic molecules of ideally lath-like shape. This approach, though, yielded controversial results [2]. In recent years, different synthetic, theoretical and simulation investigations led to the design of new mesogenic materials of eventually more complex molecular structures where the biaxial nematic ordering has been predicted and, in some cases, experimentally detected. This is the case of bent-core mesogens [4] and bent-core dimers [5], side-on liquid crystalline polymers [6], and organosiloxane tetrapodes [7]. A relevant line of research on this topic stands on the investigation of mixtures or covalently linked disk-like and rod-like mesogens, where biaxial ordering has

been predicted by theory and simulation [8] and has been the subject of recent promising synthetic works [9]. Contrary to other systems, no substantial theoretical or simulation work has been done relating the biaxial ordering detected in organosiloxane tetrapodes to the corresponding molecular structure. Recently, deuterium NMR experiments on the monomers, which constitute the organosiloxane tetrapodes, have been performed in order to contribute to the understanding of that relationship [10]. The question of correlation of the biaxial ordering of the tetrapodes with the respective molecular structure has also been addressed by the authors in a recent paper concerning complementary NMR experiments on these systems [11]. X-ray diffraction experiments on these compounds are also expected to add useful information to the problem of understanding the origin of biaxial nematic ordering of tetrapodes' systems. On this communication, structural data and deuterium NMR spectroscopy results will be discussed in order to contribute to the understanding of the correlation between the molecular structure and the biaxial nematic ordering observed on organosiloxane tetrapodes and related compounds [12].

[1] M. J. Freiser, *Phys. Rev. Lett.* **24**, 1041 (1970).
[2] G. R. Luckhurst, *Thin Solid Films* **393**
[3] See, for instance, G. R. Luckhurst, *Nature* (London) **430**, 413 (2004); D.W. Bruce, *The Chemical Record,* **4**, 10 (2004); K. Severing and K. Saalwächter, *Phase Biaxiality in Nematic Liquid Crystals, Experimental evidence for phase biaxiality in various thermotropic liquid crystalline systems,* in *Thermotropic Liquid Crystals, Recent Advances,* Springer Netherlands (2007); R. Berardi, L. Muccioli, S. Orlandi, M. Ricci and C. Zannoni, *J. Phys.: Condens. Matter* **20** (2008) and references therein.

[4] L. A. Madsen, T. J. Dingemans, M. Nakata and E. T. Samulski, *Phys. Rev. Lett*. **92**, 145505 (2004); B.R. Acharya, A. Primak, and S. Kumar, *Phys. Rev. Lett*. **92**, 145506 (2004); M. Lehmann,Shin-Woong Kang, C. Köhn, S. Haseloh, U. Kolb, D. Schollmeyer, Q. Wang and S. Kumar, *J. Mater. Chem*., **16**, 4326 (2006)

[5] C. V. Yelamaggad, S.K. Prasad, G.G. Nair, I.S. Shashikala, D.S.S Rao, C.V. Lobo , S. Chandrasekhar, *Angew. Chem. International Edition* **43**, 3429 (2004).

[6] K. Severing, K. Saalwächter, *Phys. Rev. Lett.* **92**, 125501(2004); K. Severing, E. Stibal-Fischer, A. Hasenhindl, H. Finkelmann, and Kay Saalwachter, *J. Phys. Chem. B*, **110**, 15680 (2006).

[7] K. Merkel, A. Kocot, J.K. Vij, R. Korlacki, G.H. Mehl, and T. Meyer, *Phys. Rev. Lett.*, **93**, 237801 (2004); J.L. Figueirinhas, C. Cruz, D. Filip, G. Feio, A.C. Ribeiro, Y. Frère, T. Meyer, G.H. Mehl. *Phys. Rev. Lett*; **94**, 107802 (2005); K. Neupane, S.W. Kang, S. Sharma, D. Carney, T. Meyer, G. H. Mehl, D.W. Allender, Satyendra Kumar, and S. Sprunt, *Phys. Rev. Lett*. **97**, 207802 (2006).

[8] A. Stroobants and H. N.W. Lekkerkerker, *J. Phys. Chem*. **88**, 3669 (1984); A. G. Vanakaras and D. J. Photinos, *Mol. Cryst. Liq. Cryst.* **299**, 65 (1997); A. G. Vanakaras, A. F. Terzis, and D. J. Photinos, *Mol. Cryst. Liq. Cryst*. **367**, 67 (2001); P. Palffy-Muhoray, J. R. de Bruyn, and D. A. Dunmur, *J. Chem. Phys.*, **82**, 5294 (1985);

[9] P. H. Kouwer and G. H. Mehl, J. Am. Chem. Soc. **125**, 11 172 (2003); E. Date and D.W. Bruce, J. Am. Chem. Soc. **125**, 9012 (2003); D. Apreutesei, G.H. Mehl, *Chem. Comm.* 609 (2006)

[10] M. Cardoso, J. L. Figueirinhas, C. Cruz, A. Van-Quynh, A. C. Ribeiro, G. Feio, D. Apreutesei, and G. H. Mehl, *Mol. Cryst. Liq. Cryst.* **495**, 348 (2008)

[11] C. Cruz, J. L. Figueirinhas, D. Filip, G. Feio, A. C. Ribeiro, Y. Frère, T. Meyer, and G. H. Mehl, Phys. Rev. E, **78**, 051702 (2008).

[12] D. Filip, C. Cruz, P.J. Sebastião, M. Cardoso, A. C. Ribeiro, M. Vilfan, T. Meyer, P. H. J. Kouwer, G. H. Mehl, *Phys. Rev. E* (2010), in press.

José Maria Tavares (ISEL e CFTC-UL), jtavares@cii.fc.ul.pt,

How patchy can one get and still condense? The role of dissimilar interactions in the criticality and percolation of colloids

J. M. Tavares[1,2], P. I. C. Teixeira[1,2] and M. M. Telo da Gama[2,3]

[1]Instituto Superior de Engenharia de Lisboa

Rua Conselheiro Emídio Navarro 1, P-1950-062 Lisbon, Portugal

[2]Centro de Física Teórica e Computacional da Universidade de Lisboa

Avenida Professor Gama Pinto 2, P-1649-003 Lisbon, Portugal

[3]Departamento de Física, Faculdade de Ciências da Universidade de Lisboa

Campo Grande, P-1749-016 Lisbon, Portugal

We discuss the influence of short-ranged anisotropic interactions on the thermodynamics and structure of fluids by studying a simple model of spherical particles with bonding sites. These models are relevant to understanding a range of systems, including patchy colloids (“super atoms” with controlled functionality on the scale of microns) and biopolymers. The anisotropic interactions promote aggregation (self-assembly) of the particles, which may form what is known as network fluids. These may exhibit a peculiar type of vapour-liquid condensation at extremely low densities, thereby opening up the possibility of designing “zero-density” percolated phases, which are a pre-requisite for the formation of ideal (reversible) gels. We will present detailed results for the self-assembly, thermodynamics and percolation of a model that consists of spherical particles with three bonding sites, two of type A and one of type B.

References:

J. M. Tavares, P. I. C. Teixeira and M. M. Telo da Gama, Molec. Phys. **107**, 453 (2009).

J. M. Tavares, P. I. C. Teixeira and M. M. Telo da Gama, Phys. Rev. E **80**, 021506 (2009).

J. M. Tavares, P. I. C. Teixeira and M. M. Telo da Gama, Phys. Rev. E Rapid Comm., in the press.

Fabian Vaca Chavez fvchavez@cii.fc.ul.pt, (Univ. Lisboa)
Proton multiple-quantum NMR as a tool to study reptation dynamics in polymer melts

Fabián Vaca Chávez(1) and Kay Saalwächter(2)

(1) Condensed Matter Physics Centre -University of Lisbon, Portugal
(2)Institute of Physics, Martin-Luther-University Halle-Wittenberg, Halle, Germany

In his seminal paper, de Gennes [1] propose a qualitative explanation of the polymer melts dynamics, far above the entanglement molecular weight Me, in terms of a reptative, snake-like motion of the chain through a mesh of fixed topological constraints (entanglements) set by the other chains. Here we show results from proton multiple quantum (MQ) NMR on a benchtop spectrometer [2], probing the validity of the tube model of polymer dynamics, which combines the reptation concept with the Rouse theory for unentangled chains. This fixed-tube model is insuficient for the quantitative description of actual mechanical data, and ongoing discussions focus on including dynamics of the tube itself, caused by contour-length fluctuations (CLF), arising from chain-end motions of the test chain, or constraint release (CR), arising from matrix chain motions. We also observe characteristic deviations from the tube model predictions up to high molecular weights, and show that CR processes are responsible for modified chain modes faster than actual reptation. Our results extend previous observations by neutron spin-echo spectroscopy (NSE), whose limited dynamic range poses limitations to the study of well-entangled systems.

[1] P. G. de Gennes, J. Chem. Phys., 55, 572 (1971).
[2] K. Saalwächter, Progr. NMR Spectrosc., 51, 1 (2007).

Pedro Lind plind@cii.fc.ul.pt, (Univ. Lisboa)
Recent trends for applications of Markov data analysis

We start by reviewing a general framework based in numerical procedures to derive the stochastic equation governing the evolution dynamics of one quantity of interest composing a time series. We will show how to combine this framework with variational calculus to derive additional quantities which evolve with less stochasticity than the measured physical properties of the underlying system. Further, we also show how these procedures are applied to systems with an hierarchical structure, like the cascade structure in turbulence, and to data subjected to strong

measurement noise. Applications of such methodologies for the analysis and characterization of surface topographies, rough surfaces, traffic flow and even financial market and climatological data are discussed.

Session VII

Reinhard Horst Schwarz rschwarz@fisica.ist.utl.pt(IST)

RF- plasma-assisted PLD growth of GaN and ZnO thin films

R. Ayouchi, C. Casteleiro, R. Schwarz

Departamento de Física, Instituto Superior Técnico, Lisbon and ICEMS, Lisbon

O. Conde

Departamento de Física, Faculdade de Ciências da Universidade de Lisbon, and ICEMS, Lisbon

L. Santos

Departamento de Engenharia de Materiais, Instituto Superior Técnico, Lisbon and ICEMS, Lisbon

Modern optoelectronic devices, like GaN-based green and blue semiconductor lasers, are fabricated by highly sophisticated but costly molecular-beam-epitaxy reactors (MBE) or by more conventional sputtering deposition systems. We will present our recent work on thin films of GaN and ZnO prepared by pulsed laser deposition (PLD), which is an ideal research tool due to its low cost and its high flexibility. We will discuss structural and morphological properties and try to correlate the film parameters with optical and electronic parameters.

PLD has become an important method for deposition of a large variety of thin films, including metals, semiconductors, and oxides. Examples studied at IST in recent years include GaN, ZnO, ZnN, Cu, Zn, C, and Si. As laser source we are using a ns-pulsed Nd:YAG laser system with the basic line at 1062 nm and second or fourth harmonics at 532 and 266 nm, respectively. Some processes include the presence of plasma-activated N2 or O2 background gas. This further increases the flexibility with respect to film characteristics as a function of process parameters.

As an example, we report on the structural, morphological, and optical properties of zinc oxide (ZnO) thin films obtained by reactive pulsed laser ablation of metallic Zn target in oxygen plasma atmosphere using a frequency-doubled Nd:YAG laser assisted by a 13.56 MHz radio-frequency plasma. The films were deposited in the temperature range from 400 ºC to 800 ºC and have been characterized by different methods including X-ray diffraction (XRD), Atomic Force Microscopy (AFM), Spectroscopic Ellipsometry (SE), and Photoluminescence Spectroscopy (PL). XRD measurements revealed that all the films were polycrystalline in nature. The surface roughness of the deposited films is very low at values of 2-5 nm, depending mainly on the deposition temperature. Ellipsometric parameters were fitted by using a multilayer optical model to obtain essential optical constants like refractive index and optical band gap.

We will finally try to correlate a commonly observed, but still poorly understood problem of prolonged change in photoconductivity of GaN and ZnO films observed after pulsed UV excitation. This so-called persistent photoconductivity (PPC) effect might hamper applications like fast light detectors, solid-state laser, and thin-film transistor applications.

Olinda Conde omconde@fc.ul.pt, (Univ. Lisboa)
Anomalous magnetotransport and thermoelectric properties of Fe3O4 thin films on Si(100)

O. Conde[1], M.L. Paramés[1], M.S. Rogalski[2], Z. Viskadourakis[3,4], I. Giapintzakis[4]
[1]Universidade de Lisboa, Faculdade de Ciências, Dep. Física e ICEMS, 1749-016 Lisboa
[2]Instituto Superior Técnico, Dep. Física e ICEMS, 2780-990 Taguspark Oeiras
[3]University of Crete, Materials Science and Technology Dept., 71003 Heraklion, Greece
[4]University of Cyprus, 1678 Nicosia, Cyprus

Amongst the ferromagnetic materials that are predicted to be half-metallic, magnetite (Fe_3O_4) is one of the most interesting because of its extremely high Curie temperature of ~860 K. Both properties make Fe_3O_4 a very attractive material for application in spintronic devices operating at room temperature.

Fe_3O_4 thin films were grown on Si(100) to ensure compatibility with Si technology. The pulsed laser deposition technique was used and the substrate temperature was maintained at a relatively low value of 210 ºC. The background gas consisted on a mixture of oxygen and argon.

The as-grown layers were studied *vis-a-vis* of their phase purity, stoichiometry, magnetic, electrical and magnetotransport properties. The latter show an anomalous behaviour in the temperature range 200 – 240 K where a resistivity drop and a signal reversal of the magnetoresistance are observed for the thinner films. These results will be discussed in terms of an inversion layer formed at the SiO_2/Si interface. Moreover, Seebeck coefficient data recorded on these films also show abnormal high values in the same temperature range.

Helena Cruz hcruz@cii.fc.ul.pt, (Univ. Lisboa)
Dark states in homogeneous atomic-molecular Bose-Einstein condensates

Tom Girard criodets@cii.fc.ul.pt(Univ. Lisboa)
Spontaneous vortex formation in systems with local gauge invariance

I describe various tests of the Kibble-Zurek mechanism for spontaneous topological defect formation in rapid phase transitions of superconductors, including those conducted locally, as a means of obtaining information on the formation of topological defects (cosmic strings) in higher energy cosmological scenarios.

V. Ponomarenko VPonomarenko@aim.com, (Univ. Minho)
Anyon braiding in charge transfer statistics of fractional edge-state Mach-Zehnder interferometer

We have studied the zero-temperature statistics of charge transfer between the two edges of Quantum Hall liquids with filling factors $\nu_{0,1}=1/(2 m_{0,1}+1)$ forming Mach-Zehnder interferometer. The known Bethe ansatz solution for symmetric interferometer is used to obtain the cumulant-generating function of charge at constant voltage V between the edges. Its low-V behavior can be interpreted in terms of electron tunneling, while its large-V asymptotics reproduces the m-state dynamics ($m\equiv 1+m_{0}+m_{1}$) of quasiparticles with fractional (for $m>1$) charge and anyon braiding statistics. We also analyze the transition region between electrons and quasiparticles.

Andrii Ya. Vovk ayvovk@fc.ul.pt, (Univ. Lisboa)

Magnetotransport properties of Fe/MgO Granular Multilayers

A García-García[1, 2], A Vovk[3, 4, 5], P Štrichovanec[3], J A Pardo[3, 6], C Magén[3], P A Algarabel[1, 2], J M De Teresa[1, 2], L Morellón[1, 2, 3], and M R Ibarra[1, 2, 3]

[1]Instituto de Ciencia de Materiales de Aragyn, Universidad de Zaragoza-CSIC 50009-Zaragoza, Spain
[2]Departamento de Física de la Materia Condensada, Universidad de Zaragoza, 50009-Zaragoza, Spain
[3]Instituto de Nanociencia de Aragón, Universidad de Zaragoza 50018-Zaragoza, Spain
[4]Centro de Física da Matéria Condensada da Universidade de Lisboa Campo Grande, Edifício C8, 1749-016 Lisboa
[5]Institute of Magnetism NAS of Ukraine, 36-b Vernnadsky blvd., 03142, Kyiv, Ukraine
[6]Departamento de Ciencia y Tecnología de Materiales y Fluidos, Universidad de Zaragoza, 50018-Zaragoza, Spain

The evolution of the morphology, magnetic and transport properties of Fe(*t* nm)/MgO(3.0 nm) multilayers with respect to the nominal metallic layer thickness was investigated. A comparison with existing experimental data on discontinuous metal-insulator multilayers, ultrathin epitaxial Fe films on MgO substrates and granular cermet films is made. Electrical resistivity measurements allowed us to disclose the charge transport mechanisms involved, which are closely related to the degree of discontinuity in the Fe layers. The samples with Fe thickness t<0.61 nm exhibit isotropic magnetoresistance (MR) which can be understood considering spin-polarized electron tunneling between nanometer-sized, superparamagnetic Fe grains. The MR ratio increases with decreasing temperature from ~3% at room temperature to ~10% at 30K.
It is confirmed that deposition conditions and the material composition play a crucial role in the percolation process. Nominal thicknesses of Fe layers at which infinite metallic cluster is formed and conditions for continuous Fe coverage were determined. Different methods of percolation threshold detection were analysed. We had shown that investigation of the temperature dependence of resistance in nanostructures could lead to overestimation of the percolation threshold value, while magnetic measurements alone could lead to its underestimation.

D. Leitão dleitao@fc.up.pt, (Univ. Porto)

Magnetotransport signatures on systems of nanohole arrays

D. C. LEITAOa, C. T. SOUSAa , A. APOLINARIOa, J. VENTURAa, J.B. SOUSAa , M. VAZQUEZb, J. P. ARAÚJOa
a IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal

b Instituto de Ciencia de Materiales de Madrid, ICMM -CSIC, Campus Cantoblanco 28049 Madrid, Spain

Engineering magnetic thin-films, by introducing local defects has proved to be effective in creating customized materials with designed magnetic properties [1]. Particularly interesting examples are patterned arrays of nanoholes in a magnetic film. In this case, the size of the non-magnetic inclusions alters significantly the patterned-film characteristics, when compared to a continuous one, leading to higher coercivity and remanence. Moreover, these arrays exhibit an absence of the superparamagnetic limit [1, 2], which allied to the "hardening" effect makes them strong candidates for ultra-high density recording media. As an alternative for the usual top-down patterning methods, we chose a bottom-up approach consisting of a self-assembly procedure. We employed autoorganized nanoporous alumina templates (NpATs) [2] as substrates to grow the nanohole array. The NpATs selected for this work had an average pore diameter ~ 35 nm and separation ~ 100 nm. To build the nanohole array, Permalloy (Py -Ni80Fe20) thin films were sputtered with an Ion Beam Deposition (IBD) system on top of the NpATs. Control samples were simultaneously deposited on SiO2 substrates. With the selected deposition conditions a deposition rate of 0.35 Å/s for Py target was obtained. Since the stability of the bits is related with the size of the magnetic antidots, we changed the thicknesses of the deposited Py films (2 nm < tPy < 100 nm), but keeping the density constant (~ 1010 holes/cm2). A quasi-linear dependence of the hole diameter (Dhole) on tPy was obtained: for low tPy, the magnetic film retains the shape and size of the underneath nanopores, but with increasing tPy, Dhole is reduced, until a continuous film is formed. Here, we present a detailed study on the temperature dependence (T; 20-300 K) behavior of the magnetoresistance (MR), as a function of tPy, and consequently Dhole. In plane MR measurements (longitudinal and transverse geometries) were performed for all samples and temperatures. A strong anisotropic-MR was observed (tPy >2 nm), with the exception of the smallest sample -tPy = 2 nm. Instead, this sample showed a positive-MR on both orientations. Furthermore, magnetization measurements at room temperature revealed a superparamagnetic-like curve, and transport measurements [R(T)], displayed a transition from an insulator-like (dR/dT<0) to a metallic-like (dR/dT>0) curve at 130 K. These results are consistent with a granular-type morphology film for tPy =2nm. In addition, all samples exhibited an almost linear-MR(H) behavior in high fields. This effect arises from magnetic domains that stay locked due to induced local shape anisotropy, which act as major nucleation sites. Moreover, MR magnitude increased with decreasing temperature, although its values were typically smaller than the obtained for the correspondent continuous samples (Figure 1). MR values also increased with increasing tPy, approaching the continuous regime for tPy = 100 nm. Finally, regarding the coercive field (Hc) which translates the "hardening" effect, a strong increase of Hc was observed with decreasing temperature and Dhole, ascribed to stronger magnetocrystalline and induced shape anisotropies (Figure 1).

References

[1]C. C. Wang et al., Phys. Rev. B 72, 174426-174428 (2005).
[2]Z. L. Xiao et al., Appl. Phys. Lett. 81, 2869-2871 (2002).
Figure 1: (left) Hsw dependence on T for samples with tPy of 6.5, 17, 68 and 100 nm. (right) MR maximum value dependence on T for samples with tPy of 2, 6.5, 17, 68 and 100 nm.

Session VIII

Tito Mendonca titomend@ist.utl.pt, (IST)

Phaser: the phonon laser

Nikola Paunkovic npaunkovic@googlemail.com(IST)
Information theory and Condensed Matter Physics

We review recent results on the use of quantum informational concepts in studying various problems in condensed matter physics. We focus on entanglement and fidelity and discuss the possible applications of this two quantities in characterizing phase transitions and collective behavior of macroscopic systems. We also study the measurement theory and its application to the problem of the emergence of macroscopic realism.

Entanglement represents a particular quantum form of correlations and we explore the relevance of these correlations on the critical behavior and thermodynamical properties (such as magnetic susceptibility, internal energy and pressure) of macroscopic systems. As entanglement is seen to be a crucial resource for quantum information processing, we also discuss its survival at finite temperatures and the possibility to extract it from macroscopic systems, namely spin-chains.

We show that fidelity, a measure of state distinguishability, used in quantum information, can be efficiently employed as a tool to detect some macroscopic phase transitions and we establish its relation to standard many-body properties. In particular, we summarize our results on phase diagrams of the Dickie, the XY, the Hubbard-Stoner model of itinerant magnetism and the BCS model of superconductivity, and the effects of an impurity in a superconductor film.

We discuss a novel theoretical approach to macroscopic realism and classical physics that focuses on the limits of observability of quantum effects of macroscopic objects, i.e. on the required precision of our measurement apparatuses such that quantum phenomena can still be observed, suggesting that classical laws emerge out of quantum physics under the restriction of coarse-grained measurements.

Nikolay I Polushkin nipolushkin@fc.ul.pt, (Univ. Lisboa)
Combined electron resonance in the microwave standing field:
A new design for quantum information procession devices

N. I. Polushkin 1,2

1Institute of Materials and Surfaces Science and Engineering, IST, and Laser Surface Processing Group, FCUL, Ed. C8, Campo Grande 1749-016 Lisbon, Portugal
2Institute for Physics of Microstructures, Russian Academy of Sciences, 603950 GSP-105, Nizhniy Novgorod, Russia

It is well known [1], that spin waves propagating along a surface of a ferromagnetic solid produce the microwave fields whose intensity decays away from the surface as .exp(-kz), where k is the wave number. It was recently shown [2] that the waves propagating in a lateral ferromagnetic periodic structure form a standing microwave field (SMW) whose periodicity is defined by the structure period. Here, we show that the SMW mediates intense spin-flip cyclotron resonance transitions (the combined resonance [3]) in a two-dimensional electron gas (2DEG), which is brought into close proximity with the lateral ferromagnetic structure [4]. Using a simple formalism of quantum theory of radiation, we demonstrate that the electron is able to experience the combined resonance via the Zeeman interaction with the SMW generated by an array of Fe nanostripes. Such an external potential h(r, t) having a spatial period . and angular frequency . can be considered as a perturbation of the wave function .l of an electron moving along an l-th Landau orbit in a static magnetic field. As the matrix elements of the perturbation operator exp[i(.l,.;n,-)t] n*(r)h(r). l(r)dr for a transition l.n are nonvanishing at n.l, the coordinate-dependent function h(r) allows for a nonzero rate of the transitions between the l-th and n-th Landau levels with spin rotation at the resonance that occurs when .=.l,.;n,.. To demonstrate the feasibility of the combined transitions, we consider a realistic situation where the electron is confined in a 2DEG from InGaAs. It is also shown that a novel commensurability effect arises in such a hybrid when the cyclotron diameter 2Rc is equal to the stripe width. Moreover, the performed analysis reveals that, in contrast to conventional electron spin resonance, the combined resonance excited in an engineered system such as the In0.53Ga0.47As enables a sizeable change in Rc. This finding enables exciting possibilities in spintronics, for spin-to-charge conversion in quantum computing devices [5]. Another feature is that the stray fields of the patterned elements quickly decay out of them in lateral direction. Localizing the resonant transitions via strong and localized ac fields would be a necessary step for single-electron spin manipulation in quantum information processing.
Work was supported by the Russian Foundation for Basic Research as well as by the “Ciência 2008” Program funded by the Portuguese Foundation for Science and Technology.

[1] M. G. Cottam, D. R. Tilley, “Introduction to surface and superlattice excitations” (Cambridge University Press, London, 1989).
[2] N. I. Polushkin, Phys. Rev. B 77, R180401 (2008).
[3] É. I. Rashba, Sov. Phys. Uspekhi, 7, 823 (1965).
[4] N. I. Polushkin, Phys. Rev. Lett. 103, 077201 (2009).
[5] M. Friesen et al., Phys. Rev. Lett. 92, 037901 (2004).

Posters

1. Joao Rodrigues joaonbrod@gmail.com, (Univ. Porto)
Edge reconstruction of graphene nanoribbons

JNB Rodrigues*, JMBL Santos*, NMR Peres**
* Centro de Física do Porto, Faculdade de Ciências da Universidade do Porto.
** Centro de Física, Departamento de Física da Universidade do Minho.

Graphene is a one-atom-thick sheet, made of carbon atoms arranged on a honeycomb structure (hexagons). First isolated in 2004 [1,2], it was found to exhibit high crystal quality, being very strong yet flexible and highly conductive [3].
The recently achieved advances in the manufacture of graphene single-crystals, have deepened the belief that this material will be a fertile ground for the development of diverse applications: analogical high-frequency transistors, exploiting the ballistic character of transport in nano-devices; devices based on the effects of mechanical deformation in the optical and transport properties of graphene; impermeable membranes with pores designed for specific functions; etc.. The production of graphene based reliable devices, requires a deep understanding of its optical and transport properties. As a consequence, the effects resulting from the presence of defects in graphene flakes must be understood.
One example of such defects, are those known as Stone-Wales defects (SWDs), which are sets of five and seven sided rings of carbons. Quantum chemical calculations (Density Functional Methods) have shown that when SWDs are present in graphene nano-ribbons (GNRs), the energy decreases as the defect gets closer the edge of the ribbon. Other studies have shown that the formation of SWDs at the edges of both armchair and zigzag GNRs, stabilize them energetically and mechanically [4,5]. The zigzag edge, in particular, is metastable under total reconstruction with SWDs, and a planar reconstruction spontaneously takes place at room temperature.
The study of these systems using an empirical tight-binding parameterization is a prerequisite for transport calculations. Consequently, in this talk, we will focus on the study of the electronic structure of a zigzag GNR with 5-7 SWDs at its edges (pairs of five and seven sided carbons rings), with special focus on the case of a total reconstruction of the zigzag edge with these defects.

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva and A. A. Firsov, Electric field effect in atomically thin carbon films, Science 306, 666 (2004).
[2] K. S. Novoselov, D. Jiang, T. J. Booth, V. V. Khotkevich, S. V. Morozov and A. K. Geim, Two-dimensional atomic crystals, Proc. Natl. Acad. Sci. USA 102, 10451-10453 (2005).
[3] A.H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov and A. K. Geim, The electronic properties of graphene, Rev. of Mod. Phys., Vol. 81, Jan-Mar 2009.
[4] B. Huang, M. Liu, N. Su, J. Wu, W. Duan, B. Gu and F. Liu, Quantum manifestations of graphene edge stress and edge instability: a first-principles study, Phys. Rev. Let. 102, 166404 (2009).
[5] P. Koskinen, S. Malola and H. Hakkinen, Self-passivated edge reconstruction of graphene, Phys. Rev. Let. 101, 115502 (2008).

2. Cátia Silva catiaavlis@gmail.com, (Univ. Lisboa)

Titanium dioxide co-doped with iron and cobalt

C.Silva1, A. Granadeiro Costa1, M.M.Cruz1,2 , R.C. Silva3,4 , L.C. Alves3,4 and M.Godinho1,2

1 Centro de Física da Matéria Condensada da Universidade de Lisboa, Ed. C8, Campo Grande, 1749-016 Lisboa
2 Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal
3 Laboratório de Feixe de Iões, Dep. Física, Instituto Tecnológico e Nuclear, Estrada Nacional 10, 2686-953 Sacavém, Portugal

4 Centro de Física Nuclear da Universidade de Lisboa, Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal

TiO2 is one of the most extensively studied wide band gap oxides aiming the production of diluted magnetic semiconductors by doping with magnetic ions. Doping rutile with Co or Ni using ion implantation, results in the formation of magnetic nanosized aggregates, with sizes that increase after annealing treatments in vacuum. For Fe doping, although aggregates can be found after implantation, thermal treatments in vacuum induce the formation of a ternary compound Ti-Fe-O. In this work, results for the system TiO2 co-doped with Co and Fe are presented. Single crystals of rutile were implanted with a total nominal fluence (Co+Fe) of 1´1017 cm-2 and 150 keV energy. The structural, electrical and magnetic characterizations of the samples are presented and conclusions are drawn as to the importance of the implantation order.

3. Jaime Silva silva.jaime@gmail.com, (Univ. Minho)

Effect of the fiber aspect ratio and orientation in the dielectric response of polymer-based nanocomposites

J. Silva [1,3*], R. Simoes[1,2], S. Lanceros-Mendez[3], R. Vaia [4]

1 IPC – Institute for Polymers and Composites, University of Minho, Campus de Azurém, 4800-058 Guimarães, Portugal

2 Polytechnic Institute of Cávado and Ave, Campus do IPCA, 4750-810 Barcelos, Portugal

3 Department of Physics, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal

4 Air Force Research Laboratories, Wright-Patterson Air Force Base, OH 45433-7750, USA

The addition of conducting fillers into polymeric matrices can significantly improve their electrical properties. Although heterogeneous composites have been widely investigated, the case of nanocomposites containing conductive fillers is not sufficiently understood.

In this work, the influence of fiber aspect ratio and orientation on dielectric properties of nanocomposites was studied by computer simulation, based in the graph theory framework. Simulation results are discussed and related with experimental results. We confirm that increasing the filler aspect ratio increases the dielectric constant for the same volume fraction. It is also shown that nematic sate composites show a lower dielectric constant compared to isotropic ones. Finally, it is demonstrated that for nematic state materials with different aspect ratios the dielectric constant follows a power law relative to the volume fraction.

Acknowledgements.

Effort sponsored by the Air Force Office of Scientific Research, Air Force Material Command, USAF, under grant number FA8655-06-1-3009. We acknowledge also the Foundation for Science and Technology, Lisbon, through the 3° QuadroComunitario de Apoio, the POCTI and FEDER programs, and the PTDC/CTM/69316/2006 grant. JS thank the FCT grant SFRH/BD/60623/2009

4. Fátima Cerqueira fcerqueira@fisica.uminho.pt(Univ. Minho)
Erbium emission of nc-Si:Er grown by r.f. sputtering. Effect of crystal size and crystalline volume fraction on PL emission

M. F. Cerqueira[1], E. Alves[2], A. Kozanetkhy[3], P. Alpuim[1]

[1] Departamento de Física, Universidade do Minho, Campus de Gualtar 4710-057 Braga, Portugal

[2] Instituto Técnico Nuclear ITN, EN 10, 2686-953, Sacavém, Portugal

[3]Polish Academy of Sciences, Institute of Physics, PL-02668, Warsaw, Poland

Erbium-doped crystalline silicon, c-Si:Er, is a possible alternative to achieve efficient light emission from silicon. To overcome the 1.54 μm-back energy transfer from Er^{3+} ions to the c-Si matrix, the use of a high bandgap dielectric matrix, where Si nanocrystals are embedded as sensitizers for the Er^{3+} photoluminescent centers, has been reported in literature. Hydrogenated nanocrystalline silicon (nc-Si:H), consisting of silicon nanocrystals embedded in a higher optical bandgap amorphous-Si matrix, is expected to behave in much the same way, with the advantage that electrically pumped photoluminescence (PL) would be possible, since it is easy to inject and drift electrons and holes across the material.

In this work erbium-doped low-dimensional Si films (nc-Si:Er) with different microstructures were grown by reactive magnetron sputtering on glass substrates by varying the deposition parameters. Their structural and chemical properties were studied by micro-Raman and Rutherford backscattering spectroscopy, respectively. In this contribution the Erbium emission is studied as a function of nanocrystalline fraction and crystal sizes. We will discuss the temperature dependence of the Er^{3+} emission as also the explanation of the low Er active maximum fraction due to the fact that these ions are not enough close to the neighboring Si nanocrystals.

5. Marta Jussara Souza da Rocha msrocha@fc.ul.pt (Univ. Lisboa)
Magnetic nanoparticles of nickel and iron oxides

M.J.S. Rocha[1], M.D. Carvalho[2], M.M.Cruz[1,3] and M.Godinho[1,3]

[1] Centro de Física da Matéria Condensada da Universidade de Lisboa, Ed. C8, Campo Grande, 1749-016 Lisboa
[2] CCMM / Dep. de Química e Bioquímica, Faculdade de Ciências, Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal
[3]Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal

Aiming the future production of magnetic nitrates, nickel and iron oxide nanosized particles were produced using two distinct routes: the sol-gel combust method and the hydrothermal method. Citric acid, urea and β-lanina were used as precursors for the combustion, in the search for powders with smaller particle size.

Structural characterization using X-ray diffraction (XRD) allowed phase identification and the determination of the particles average diameter. Magnetic characterization was carried out using a SQUID magnetometer in the temperature range between 2 K and 400 K, under magnetic fields up to 5.5 T. For the nickel oxide particles, superparamagnetic behavior was observed and a complete characterization of the distribution of volume sizes was done. The comparison between the samples obtained with different methods and precursors determined the best synthesis method for the oxide particles production.

6. Joao Ventura joventur@fc.up.pt, (Univ. Porto)
Temperature dependent transport properties of MgO-based ultra-thin magnetic tunnel junctions: experiment and modeling

J. M. Teixeira, J. Ventura, J. P. Araújo, J. B. Sousa, P. Wisniowski, and P. P. Freitas

Magnetic tunnel junctions (MTJs), constituted by two ferromagnetic (FM) layers separated by an insulating barrier, are currently used as magnetic sensors in high density recording media. The characteristics of the tunnel junctions implemented in read heads include a low resistance-area product (R × A), to achieve a high readout speed, and a high enough

sensitivity to read the ever smaller magnetic bit. To achieve the desired R × A-values, the thickness of the insulating barrier is decreased to less than one nanometer, towards a few atomic planes thick. This leads to the possible existence of metallic paths across the insulating barrier (pinholes), with consequences in device reproducibility, performance and reliability. Recently, tunnel junctions with crystalline MgO(001) barriers displaying very large tunnel magnetoresistive (TMR) ratios were successfully fabricated, opening new opportunities to develop read heads for ultrahigh density hard drives. The large TMR ratio of crystalline MgO tunnel junctions arises from the different symmetry-related decay rates of the Bloch waves for majority and minority spin channels. MTJs with tunnel magnetoresistance above 50% and R × A as low as 0.4 $\Omega\mu m^2$ were recently obtained using thin MgO barriers.[1] However, a significant TMR-decrease is usually observed with decreasing MgO thickness,[2] showing the importance of studying the impact of pinholes on the magneto-transport properties of ultra-thin magnetic tunnel junctions. To probe the absence of pinholes in MTJs one usually uses the three applicable Rowell criteria. However, both the exponential dependence of resistance with insulator thickness and the non-linear current-voltage characteristics were found to be non-reliable even in high resistance tunnel junctions (R × A $\geq$ 1 $k\Omega m^2$).[3] On the other hand, the third criteria [the weak insulating-like temperature dependence of the electrical resistance (dR/dT<0)], although insensitive to the presence of few or small pinholes in low resistance MTJs ($\leq$ 10 $\Omega\mu m^2$),[4] can be used to probe if sizeable pinholes are present in the barrier.[5]

Here we study the temperature dependence (300-20 K) of the transport properties of low resistance magnetic tunnel junctions with an ultra-thin MgO barrier (7.5 Å). Our samples display R × A $\geq$ 40 $\Omega\mu m^2$ and TMR ~ 60-75% at room temperature. Temperature dependent electrical resistance measurements [R(T)] allowed us to observe different behaviors depending on the MTJ-magnetic state. The studied samples showed positive dR/dT for the parallel (P) state, indicating a metallic-like behavior, so that pinholes are already present in the barrier. However, in the antiparallel (AP) state, the R(T) curves exhibit a mixed character, with dR/dT negative at sufficiently high temperatures but changing to positive at low temperatures. These results show an interesting competition between tunnel and metallic transport in the studied samples. In order to understand this transport behavior, we propose a simple model of two conducting channels, metallic and tunnel, acting in parallel. We assume a linear temperature variation of the electrical resistance for both conducting channels, as observed experimentally over a broad temperature range. The model also takes into account the experimentally observed dependence of the linear coefficients on the MTJ-magnetic state (parallel and antiparallel). According to the model, the sign of the dR/dT derivative does not illustrate the dominant conductance mechanism and the crossover temperature (T^*) at which dR/dT changes sign in the AP state depends strongly on the linear temperature coefficients. Fittings performed to the experimental R(T) data, reproduce the data quite well, illustrating the validity of the model.

[1] Y. Nagamine *et al*, Appl. Phys. Lett., **89** (2006) 162507.
[2] K. Tsunekawa *et al*, Appl. Phys. Lett., **87** (2005) 072503.
[3] B. J. Jönsson-Åkerman *et al*, Appl. Phys. Lett., **77** (2000) 1870.
[4] J. Ventura *et al*, J. Phys. Cond. Matt., **19** (2007) 176207.
[5] J. Ventura *et al*, Appl. Phys. Lett., **90** (2007) 032501.

7. Hugo Gonçalves hgsilva@fc.up.pt, (Univ. Porto)

Transport Processes in Metal-Insulator Granular Layers

Y. G. Pogorelov,[1] J. F. Polido,[2] H. G. Silva[1,3]

[1]IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal; [2]University of Strathclyde, 76 Southbrae Drive, Glasgow, G13 1PP, Scotland, United Kingdom; [3]Center of Electronic, Optoelectronics and Telecommunications (CEOT), Universidade do Algarve, Campus de Gambelas, 8005-139 Faro, Portugal

The tunnel transport processes are considered in a square lattice of metallic nanogranules embedded into insulating host to model current-in-plane conduction in a real metal/insulator granular layer. Based on a simple model with three possible charging states (± or 0) of a granule and three kinetic processes (creation or recombination of a ± pair, and charge translation) between neighbor granules, the mean-field kinetic theory is developed. This approach generalizes the well known works of Sheng and co-authors [1, 2] that only consider the last process. We consider the interplay between granule charging energy and temperature and between the applied electric field and the Coulomb fields by non-compensated charge density in the ensemble of charged granules. The resulting charge and current distributions are found to differ essentially in the free area (FA) between the contacts and in the contact areas (CA) with respect to macroscopic metallic contacts on a granular layer. It is shown that generation of long-ranged Coulomb fields completely prevents charge accumulation in FA, resulting in essentially ohmic conduction. On the other hand, formation of image charges in the contacts reduces the effect of non-compensated charge density to short-ranged dipolar fields, making possible important charge accumulation in CA. Approximate analytic solutions found for this region display two principal conduction regimes: ohmic law below a certain crossover voltage V_0 and a non-ohmic $I \sim V^{3/2}$ law above this crossover. Using the model parameters related to recent experimental work [3] (with $V_0 \sim 5$ V) we estimate that the CA resistivity should be about two orders of magnitude higher than that for FA, so the overall transport is controlled by the CA.

Actually, the two regimes indicated for CA are in a reasonable agreement with experiments [3].

[1] P. Sheng and B. Abeles, Phys. Rev. Lett. 28, 34 (1972).
[2] P. Sheng, B. Abeles and Y. Aire, Phys. Rev. Lett. 31, 44 (1973).
[3] H. G. Silva, H. L. Gomes, Y. G. Pogorelov, L. M. C. Pereira, G. N. Kakazei, J. B. Sousa, J. P. Araújo, J. F. L. Mariano, S. Cardoso, and P. P. Freitas, J. Appl. Phys. 106, 113910 (2009).

8. Teresa Monteiro Seixas tmseixas@fc.up.pt, (Univ. Porto)
Analysis of the magnetic specific heat of Gd4Co3 compound

T. M. Seixasa,*, M. A. Salgueiro da Silvaa, O. F. de Limab, J. Lopezb, H. F. Braunc and G. Eskac

aDepartamento de Física da Universidade do Porto, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal

bInstituto de Física Gleb Wataghin, Universidade Estadual de Campinas, 13083-970, Campinas, SP, Brazil

cPhysikalisches Institut, Universitaet Bayreuth, D – 95440 Bayreuth, Germany

The magnetic contribution () to the specific heat of Gd4Co3 was determined using a new method that fits the electronic specific heat coefficient (.) and the Debye temperature (.D) by constraining the resulting magnetic entropy () to saturate at temperatures far above the Curie temperature (TC). exhibits a low temperature bump originated from thermal excitation of gapped spin waves, which is responsible for pronounced peaks, at . 35 K, in both and the temperature derivative of the magnetic contribution to electrical resistivity (). Apart from the vicinity of TC, an excellent global correlation was found between and . Our results provide strong support to the consistency of the new method proposed for the determination of and rule out any major role of short-range order on Gd moments or d-electron spin fluctuations effects in the paramagnetic phase A comparative analysis with other methods used in similar compounds points to the need for a better evaluation of in such compounds, especially in the magnetically ordered phase, where a deficient evaluation of has a larger impact on the curve.

9. Lígia Silva silva.lc@gmail.com, (IST)
Synchronization of macrospins in a linear array

Lígia Silva, Paul Horley, Vítor Rocha Vieira and Vitalii Dugaev

The synchronization of several spin valves is important for the applications, in order to increase the power output. The synchronization of an array of macrospins is studied performing numerical simulations

using the Landau-Lifshitz-Gilbert equation, including the Slonczewski spin torque term. The parameter space is explored to optimize the synchronization.

10. A. Costa acosta_df@netcabo.pt, (Univ. Lisboa)

Nitrogen and Argon doped Zinc Oxide

A.R. Granadeiro Costa1, C.Silva1, M.M.Cruz1,2, R.C. Silva3,4, L.C. Alves3,4 and M.Godinho1,2
1 Centro de Física da Matéria Condensada da Universidade de Lisboa, Ed. C8, Campo Grande, 1749-016 Lisboa
2 Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal
3 Laboratório de Feixe de Iões, Dep. Física, Instituto Tecnológico e Nuclear, Estrada Nacional 10, 2686-953 Sacavém, Portugal
4 Centro de Física Nuclear da Universidade de Lisboa, Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal

Zinc oxide has long been considered a suitable candidate for diluted magnetic semiconductors (DMS), materials combining both spin coherence and charge transport properties. In the last years, several studies involving doping with magnetic and non magnetic ions have shown that defects influence the magnetic properties of the oxide. There are several ways to create defects in a lattice (ionic implantation, thermal annealing, electron irradiation, film growth) however there is not yet a clear understanding of their role in the magnetic behaviour of the host.

Nitrogen was one of the originally proposed dopants to achieve p-type conductivity and till now no other element has proved to be a better alternative. Substitutional N on oxygen sites was identified as the main acceptor impurity and associated to a deep acceptor level around 0.2 eV in ZnO.

In this work we implant argon and nitrogen in ZnO single-crystals to compare the influence of the two different non magnetic elements in the magnetic and electrical behaviour of the zinc oxide. Single crystalline samples are essential to the study of electrical resistivity since they allow avoiding grain boundary effects.

Structural, magnetic and electrical results are presented and discussed.

11. Nelson Bernardino nelson.bernardino@mf.mpg.de (Max Planck Stuttgart)
The interaction of interfaces with substrate

A thin layer of liquid forms at a substrate exposed to a vapour.
The form of the interaction between the liquid-vapour interface with the underlying substrate is of fundamental importance in a wide range of problems involving interfaces in condensed matter. We show a specific example, in the context of the physics of wetting, in which the effective interaction can be calculated exactly and this result is used to solve several problems that have been open for more than 20 years.

12. Rui Borges rpborges@fc.ul.pt (Univ. Lisboa)
Magnetic properties of BaFeO3 thin films deposited by pulsed injection MOCVD

B. Ribeiro[a], R. P. Borges[a], P. C. Ferreira[b], M. Godinhoa[c]

[a]Centro de Física da Matéria Condensada da Universidade de Lisboa, Ed. C8, Campo Grande, 1749-016 Lisboa.

[b]Departamento de Engenharia Cerâmica e do Vidro, CICECO, UniversidadedeAveiro, CampusUniversitário deSantiago, 3810-193 Aveiro, Portugal.

[c]Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal.

Thin film deposition allows the stabilisation of structural phases that are not accessible in bulk form. This provides an important route to tailor the properties of magnetic materials to the requirements of different applications. Bulk $BaFeO_{3-\delta}$ is known to assume different crystal structures (hexagonal, cubic, tetragonal, orthorhombic, monoclinic) depending on the oxygen stoichiometry. For $\delta < 0.25$ the compound has a hexagonal structure and is paramagnetic above 250 K while for higher values of δ it can assume the cubic structure and show magnetic ordering at room temperature. In order to explore their structural and magnetic properties, thin films of $BaFeO_3$ were grown by Pulsed-Injection Metal Organic Chemical Vapour Deposition (PI-MOCVD) on cubic $SrTiO_3$ and $LaAlO_3$ single crystal substrates using different deposition conditions. The films were characterized in the as deposited state and after a thermal treatment in oxygen atmosphere, using X-Ray diffraction, atomic force microscopy and SQUID magnetometry. By tuning the deposition conditions, notably the substrate temperature and the relative concentrations of Ba and Fe precursors, it was possible to obtain films

that have a cubic structure, are insulating and show antiferromagnetic properties at room temperature.

13. Elsa Lopes eblopes@itn.pt (ITN)
The search for new materials for thermoelectrical applications

E.B. Lopes[1], A.P. Gonçalves[1], O. Rouleau[2], C. Godart[2]

[1]Dep. Chemistry, ITN/CFMC-UL, Estrada Nacional 10, P-2686-953 Sacavém, Portugal

[2] Lab. de Chimie Metallurgique des Terres Rares, ISCSA-CNRS UPR209, Thiais, France.

Thermoelectric devices can convert reversibly thermal energy into electrical energy. The thermoelectrical efficiency of a device is mainly determined by the adimensional parameter ZT (figure of merit). Present thermoelectrical devives are based on Bi2Te3 and Si-Ge phases and have ZT values around 1, which correspond to efficiencies of the order of 10% and are still low to compete with other environment friendly energy sources. On the other hand this devices easily allow the conversion of waste heat into energy. The identification, synthesis and characterization of new thermoelectrical systems with higher figure of merit is fundamental to consolidate these systems as viable environment friendly energy sources.

This work presents the study of the family of semiconducting glasses with $Cu_{x+y}Ge_{20-x}Te_{80-y}$ ($0 \leq x \leq 20$; $0 \leq y \leq 10$) general composition. The samples of this family have been prepared by melt spinning and used to test the possibility of obtaining conducting glasses for thermoelectric applications. These amorphous materials have very a large Seebeck coefficient that is relatively insensitive to changes in composition but as the Cu content is increased they become progressively more conducting. They also possess a small thermal conductivity, as expected, because of their intrinsic disordered nature. The transport properties will be discussed with the help of hopping models as expected for amorphous semiconductors. ZT values of the order of 0.2 [1,2] were obtained in an element of this family, indicating chalcogenide glasses as potential candidates for high performance thermoelectric materials.

References

1- A.P. Gonçalves, E.B. Lopes, E. Alves, N.P. Barradas, N. Franco, O. Rouleau, C. Godart, Book Series: NATO Science for Peace and Security Series B - Physics and Biophysics, eds. V. Zlatić, A. Hewson, Springer, 2009, pp. 51-67.
2- A.P. Gonçalves, E.B. Lopes, O. Rouleau, C. Godart, Journal of Materials Chemistry, J. Mater. Chem. 2010, DOI: 10.1039/B908579C

14. Célia Tavares de Sousa celiasousa@fc.up.pt (Univ. Porto)
Pulsed electrodeposition of metal nanowires in nanoporous alumina templates

C.T. Sousa[1], D.C. Leitão[1], A.M.Pereira[1],A.Apolinário[1], M.P. Proença[1], J. G. Correia[2], J. Ventura[1], J.P. Araújo[1]*

[1]IN-IFIMUP and Dep. Física, Rua do Campo Alegre 687, 4169-007 Porto, Portugal

[2]ITN, Estrada Nac. N10, Apartado 21 – 2686-953 Sacavém, Portugal

The great advances in nanoscience and nanotechnology in the last decade have lead to the development of new platforms where all physical properties like size, porosity, geometry and surface functionalization can be controlled at the nanoscale. The research devoted to this field is pushed by the potential applications offered by such structures in several areas, ranging from spintronics to nanomedicine. Particularly, high aspect ratio inorganic nanoparticles have arouse great interest and shown many potentialities. Among the different approaches to the fabrication of these high aspect ratio nanoparticles, alumina template-based synthetic methods have received considerable attention due to their several unique structural properties, such as controllable pore diameter, extremely narrow pore size distribution, and an ideally cylindrical shape. Especially, template electrodeposition has been proved to be an effective way to fabricate metallic nanowires. Until now, three different methods have been developed to obtain uniforme and complete filling of template pores by electrodeposition: direct current (DC), alternating current (AC) and pulsed electrodeposition (PED). The PED method usually consists on the application of DC pulses with square or other complex electronic waves. Contrary, to DC deposition, AC deposition and PED can be performed if a thin barrier layer is present in the pore bottom. Since aluminium substrate and alumina barrier layer do not need to be removed for AC deposition and PED, pore filling is simple and nanowires with very small length can be fabricated. PED can thus be a reliable alternative method for the deposition of metals into high aspect ratio forms. However, pre-treatment of the alumina template before PED is needed because the resistance during the electrodeposition varies depending on the thickness of the bottom of the pores. This influences the deposition behaviour, since electrodepostion preferably occurs in those pores exhibiting a thinner (less resistive) barrier layer. Therefore, the barrier layer is thinned by decreasing the voltage at the end of the anodization process. The nanowires are straightforwardly electrodeposited on the bottom of nanohole and the procedure is very simple.

In this work we will describe the PED stages of growth of metallic nanowires into anodic nanoporous alumina. After a two step anodization process, an exponential voltage was applied leading the formation of dendrites at the pore bottom. Metal deposition was achieved without removing the aluminum substrate because a PED method in the microsecond range with an intermittent asymmetric square pulse was used. We further present an optimization of the type and the thickness of the barrier layer to control the homogeneity and the length of the nanowires.

15. André Espinha acmespinha@gmail.com, (Univ. Porto)
Polar nano-structures for technical applications

A. Espinha [1], S. Patrício[2], A. Almeida[1], C. Freire[2], J. Agostinho Moreira[1], C. T. Sousa[1], J. P. Araújo[1]

[1] *Department of Physics, Faculty of Science, University of Porto, Portugal.*

[2] *REQUIMTE/Department of Chemistry, Faculty of Science, University of Porto, Portugal.*

In the last decades, polarizable materials have drawn huge interest due their applications to emergent technologies. Unlike inorganic materials, organic-based systems have quite reduced environmental impact, enabling the development of biodegradable electronics and photonics.

The general approach for producing organic polar materials (OPM) is to start from polar molecular units [1]. Contrarily, the materials used in this work are based on supramolecular chains of non-polar units.

In a first step, the organic compounds were obtained by precipitation after mixing methanolic solutions of the precursor molecules. After the processing, they were characterized by different experimental techniques: FTIR and Raman spectroscopy, UV/VIS spectroscopy, dielectric spectroscopy, and measurement of both thermal depolarized stimulated current and polarization inversion.

In a second step, the phenazine/chloranilic acid-based system ($PhzH_2ca$) was chosen to be immobilized in nanoporous alumina membranes [2]. The temperature dependence of the dielectric permittivity reveals that the transition temperature undergoes a shift of more than ~80 K - to 325 K, wherein the maximum of the anomaly corresponds to an increase of ~160% relative to the value measured at low temperatures. This result provides that immobilization in nanoporous alumina membranes is a promising method for enhancing polar properties of organic polar co-crystals, making them readily usable in technology, particularly as radiation sensors or actuators, at room temperature.

References:

[1] S. Horiuchi et al (2005), *Ferroelectricity near room temperature in co-crystals of nonpolar organic molecules*, Nature Materials, vol. 4.

[2] S. Horiuchi (2008), *Organic Ferroelectrics*, Nature Materials, vol. 7.

16. Pedro Ribeiro ribeiro@cfif.ist.utl.pt, (IST)
U(1) slave-particle study of the finite-temperature doped Hubbard model in one and two dimensions

One-dimensional systems have unusual properties such as fractionalization of degrees of freedom. Possible extensions to higher dimensional systems have been considered in the literature. In this work we construct a mean-field theory of the Hubbard model taking into account a separation of the degrees of freedom in a way close to the one-dimensional case and study the finite-temperature phase diagram for the Hubbard chain and square lattice.

17. Ricardo Guimaraes Dias rdias@ua.pt, (Univ. Aveiro)
Critical hybridization for the Kondo resonance in gapless systems

R. G. Dias, Lídia del Rio, A. V. Goltsev

We study the Kondo resonance in a spin-1/2 single impurity Anderson model with a gapless conduction band using the equation of motion approach in

order to obtain the impurity spectral function. We study two different scenarios for gapless systems: a purely power-law energy dependence of the density of states or a constant density of states with a gapless behavior near the Fermi level. We demonstrate that strong electron-electron correlations lead to a sharp peak in the impurity spectral function in the case of a large exchange coupling ($J>J_{c}$) or equivalently, a strong hybridization ($V>V_{c}$). This Kondo-like peak emerges much below the Fermi level in the case of a strongly depleted density of states. These results are compared with the ones from renormalization group approaches.

18. M.A.N. Araújo mana@uevora.pt (Univ. Évora)

Andreev reflection between a normal single-band metal and a Fe-pnictide superconductor

M. A. N. Araújo(1,2) e P. D. Sacramento(1)
(1) CFIF, Instituto Superior Técnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
(2) Departamento de Física, Universidade de Évora, P-7000-671, Évora, Portugal

The problem of Andreev reflection between a normal single-band metal (N) and a multiband superconductor (MBS) is addressed. The splitting of the incident electron's probability amplitude among several conduction channels in the MBS is the same quantum mechanical problem as in a quantum waveguide. The appropriate matching conditions for the wave function at the interface are established on the basis of an extension of quantum waveguide theory to the N/MBS boundary.
A Fe-pnictide superconductor is specifically considered, in the framework of a recently proposed effective two-band model and various pairing scenarios. Andreev bound states (ABS) emerge in the sign-reversed s-wave scenario, due to interference effects between the bands. An unusual feature of these ABS is that they occur at a finite energy above the Fermi level, which disperses with the electron's transverse momentum. The interference effects may also suppress the conductance at certain energies.

19. J. G. Barbosa jbarbosa@fisica.uminho.pt (Univ. Minho)

Barium titanate thin films deposited by electrophoresis on p-doped Si(001) substrates

J.G. Barbosa[1], M.R. Pereira[1], J.A. Mendes[1,2], B.G. Almeida[1]

[1]Dep. de Física, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal.

[2]ESEIG, IPP, Rua D. Sancho I, 981, 4480-876 Vila do Conde, Portugal.

In recent years, barium titanate ($BaTiO_3$) thin films have been the subject of intense studies, since it is a good candidate for application on multilayer capacitors, dynamic random access memories or tunable microwave devices. The need for the integration of $BaTiO_3$ with semiconductor nanoscopic structures or devices makes it important to develop high quality and reliable $BaTiO_3$ thin films on semiconductor substrates. Electrophoretic deposition (EPD) is a versatile technique that has been used for the production of functional ceramic thin films. In this technique an electric field is applied on a suspension of charged particles (sizes < 30 nm) that migrate and are deposited on an electrode. Electrophoresis can be applied with different materials and combinations of materials and has the ability to be scaled-up to large product volumes and sizes. Here, $BaTiO_3$ thin films have been deposited by electrophoresis on p-doped Si(001) substrates and their structure was studied by X-ray diffraction (XRD) and Raman spectroscopy.

The $BaTiO_3$ nanoparticles, for the suspension, were prepared by the sol-gel method, using barium diethoxide and titanium (IV) isopropoxide as precursors. They were then dispersed on an EGMME+Acac solution and a voltage was applied in order to deposit the films. The as-deposited films were polycrystalline and composed by barium titanate with the cubic structure. Their grain size, as measured from the X-ray diffraction peak width, was 13 nm. Subsequently, to promote grain growth and the stabilization of the tetragonal ferroelectric phase, the films were annealed at high temperatures. For the films annealed at 600ºC during 2h, the XRD and Raman results presented peaks characteristic of the tetragonal-$BaTiO_3$ structure. The calculated *a* and *c* lattice parameters, from the XRD peak positions, were similar to the corresponding bulk values. The influence of the preparation conditions on the structural and dielectric properties of the deposited $BaTiO_3$ thin films will be presented

20. Andrea Parisi parisia@ptmat.fc.ul.pt, (Univ. Lisboa)

Pattern dynamics in eutectic solidification

Eutectic alloys are widely used in the metallurical industry and have been studied for years from metallurgists. When directionally solidified they form patterns of two distinct solid phases, organized spatially as lamellar or rod arrays, that influence the mechanical properties of the final solidified samples. Thus, predicting what kind of structures arise depending on solidifying conditions has been a relevant quest for industry. It is only in recent years that physicists have been more deeply involved thanks to the discovery of transparent organic eutectic alloys which allow to observe the dynamical evolution of the solidification patterns in real time. Additionally, the development of performant quantitative simulation methods based on the phase field approach has provided the numerical tools for a deep investigation of the issues involved in these processes. From the point of view of pattern forming systems, the observed patterns are similar to those of other pattern forming systems such as reaction diffusion, however there are a few distinct features which seem to be specific of this particular system. I will review the basis of eutectic solidification as well as the

phase field method for simulations, and illustrate the major results and insights obtained so far.

21. Pedro Patrício pedro.patricio@dem.isel.ipl.pt, (ISEL)
COMPLETE WETTING TRANSITIONS OF NEMATIC LIQUID CRYSTALS ON A STRUCTURED SUBSTRATE

P. Patrício(a,b), C.-T. Pham(c) and J. M. Romero-Enrique(d)
(a) Instituto Superior de Engenharia de Lisboa, R. Conselheiro Emídio Navarro 1, 1949-014 Lisboa Codex, Portugal;
(b) Centro de Física Teórica e Computacional da Universidade de Lisboa, Av. Prof. Gama Pinto 2, 1649-003Lisboa Codex, Portugal;
c) Laboratoire d'Informatique pour la Mécanique et les Sciences de l'Ing nieur, CNRS-UPR 3251, Université Paris-Sud 11, BP 133, F-91403 Orsay Cedex, France
(d) Departamento de Física Atómica, Molecular y Nuclear, Area de Física Teórica, Universidad de Sevilla.

It is known that the wetting behaviour of a fluid is deeply altered in the presence of rough or structured substrates. We will first review some simple considerations about isotropic fluids and rough substrates, and then we will generalize Wenzel's law, which assigns an effective contact angle for a droplet on a rough substrate, when the wetting layer has an ordered phase, like a nematic. We estimate the conditions for which the wetting behaviour of an ordered fluid can be qualitatively different from the one usually found in a simple fluid. To particularize our general considerations, we will use the Landau-de Gennes mean field approach to investigate theoretically and numerically the complete wetting transition between a nematic liquid crystal and a periodic triangular structured substrate. For this particular microstructured substrate, we report the emergence of disclination lines in the nematic phase, characterized by non-half-integer winding numbers . These topological defects nucleate in the wedges and apexes of the substrate. As a consequence, the Berreman expression for the elastic contribution to the free energy density breaks down, as an additional term proportional to q ln q appears, q being the wavenumber associated with the substrate periodicity.

22. Nuno Silvestre nunos@cii.fc.ul.pt, (Univ. Lisboa)
Islands in free standing smectic C films

N. M. Silvestre1, 2, P Patrício1, 3 and M M Telo da Gama1, 2
1 Centro de Física Teórica e Computacional and
2 Departamento de Física da Faculdade de Ciências, Universidade de Lisboa, Avenida Professor Gama Pinto, 2, P-1649-003 Lisboa Codex, Portugal.
3 Instituto Superior de Engenharia de Lisboa Rua Conselheiro Emídio Navarro 1, P-1949-014 Lisboa, Portugal.

Colloidal dispersions in liquid crystals are different from the ordinary colloids due to the long-range orientational order of the liquid crystal molecules. In addition, colloidal particles present complex interactions that have a long-range dipolar or quadrupolar profile that are an important feature of the self-organisation into supermolecular structures specific from colloidal liquid crystals. The structures observed in

experiments are stabilized by the presence of topological defects that induce complex short-range repulsions. The study of such interactions in films is important for a complete understanding of three dimensional colloidal dispersions in liquid crystal. We present some of the work done on dipolar and quadrupolar interactions of colloidal particles in smectic C films.

23. Frank Raischel frank.raischel@googlemail.com, (Univ. Lisboa)
Fiber bundle models for shear failure and plasticity

The fracture and failure of fiber reinforced materials such as wood, reinforced concrete, GFRP (glass fiber reinforced polymers) or CFRP (carbon fiber reinforced polymers) is considerably determined by the disordered properties of these materials and their constituents. A comprehensive understanding of their degradation and failure therefore requires the inclusion of statistical methods.
The class of fiber bundle models (FBM) holds an eminent position among these statistical approaches, due to their ability to describe the stochastic nature of heterogeneous materials, and the dynamical rearrangements upon partial failure. In their simplest representation, the classical FBM models a bundle of parallel fibers under longitudinal strain, where each fiber is characterized by modulus of elasticity and a statistically sampled failure threshold. Under increasing load, individual fibers fail and redistribute their load upon neighboring fibers according to a load sharing law, thus potentially triggering avalanches of further failures.
I will describe how the use of fibre bundle models helps to understand the failure of fiber reinforced materials under shear, and how the classical FBM can be modified to describe the appearance of plasticity. Fiber bundle models also allow to capture the appearance of statistical precursors of imminent failure. In addition, I will highlight how to improve already existing fibre bundle models for continuous damage, in order to account for the failure of materials with a pronounced hierarchical setup. Finally, an outlook on recent developments will be given.

24. Pedro Sebastião pedro.jose.sebastiao@ist.utl.pt, (IST)
NMR relaxation study of molecular dynamics of liquid crystalline organosiloxane tetrapodes and octapodes

D. Filip[a, b], A. Van-Quynh[a], C. Cruz[a, c], P.J. Sebastião[a, c], M. Cardoso[a], A. C. Ribeiro[a, c], M. Vilfan[d], T. Meyer[e], P. H. J. Kouwer[e], G. H. Mehl[e]

[a]CFMC-UL Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal

[b]"Petru Poni" Institute of Macromolecular Chemistry, Aleea Gr. Ghica Voda 41A, 700487-Iasi, Romania

[c]IST-UTL, Av. Rovisco Pais 1049-001 Lisboa, Portugal

[d]Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

[e]Dep. Chemistry, University of Hull, Cottingham Road, Hull HU6 7RX, United Kingdom

Proton NMR relaxation measurements were carried out on liquid crystalline organosiloxane tetrapodes with end-on and side-on mesogenic groups, and on an organosiloxane octapode with side-on mesogenic groups. In addition, a liquid crystal monomeric analogue of one of the tetrapodes was also studied. The systems present different mesophases (e.g. nematic, smectic C phases, and columnar phases).[1-4] NMR relaxometry of the multipode systems yields T_1^{-1} dispersions clearly different from those of conventional calamitics. The influence of molecular tendency to form interdigitated structures is evidenced by the frequency dependent relaxation rate in the isotropic phase – indicating the presence of ordered clusters far above the phase transition – and by the diminished role of molecular self-diffusion in the ordered phases. Collective motions detected by proton NMR relaxometry at low frequencies are clearly associated with the structure of the studied mesophases.

1. K. Merkel, A. Kocot, J.K. Vij, R. Korlacki, G.H. Mehl, and T. Meyer, *Phys. Rev. Lett.* **2004**, *93*, 237801

2. D. Filip, C. Cruz, P.J. Sebastião, A. C. Ribeiro, T. Meyer, G. H. Mehl, *Mol. Cryst. Liq. Cryst.* **2005**, *436,* 17

3. D. Filip, C. Cruz, P. J. Sebastião, A. C. Ribeiro, M. Vilfan,T. Meyer, P. H. J. Kouwer, G. H. Mehl, *Phys. Rev. E*, **75**, 11704(2007)

4. D. Filip, P. J. Sebastião, C. Cruz, A. C. Ribeiro, M. Vilfan, T. Mayer, P. H. J. Kouwer, G. Mehl. Accepted in *Phys. Rev. E*

25. Ganna Rozhnova a_rozhnova@cii.fc.ul.pt (Univ. Lisboa)

Cluster approximations for infection dynamics on random networks

Ganna Rozhnova, Ana Nunes

In this paper, we consider a simple stochastic epidemic model on large regular random graphs and the stochastic process that corresponds to this dynamics in the standard pair approximation. Using the fact that the nodes of a pair are unlikely to share neighbors, we derive the master equation for this process and obtain from the system size expansion the power spectrum of the fluctuations in the quasi-stationary state. We show that whenever the pair approximation deterministic equations give an accurate description of the behavior of the system in the thermodynamic limit, the power spectrum of the fluctuations measured in long simulations is well approximated by the analytical power spectrum. If this assumption breaks down, then the cluster approximation must be

carried out beyond the level of pairs. We construct an uncorrelated triplet approximation that captures the behavior of the system in a region of parameter space where the pair approximation fails to give a good quantitative or even qualitative agreement. For these parameter values, the power spectrum of the fluctuations in finite systems can be computed analytically from the master equation of the corresponding stochastic process.

26. Maria Isabel Fialho Cabaco isabel@cii.fc.ul.pt, (IST)

COMPLEX FORMATION OF CARBON DIOXIDE WITH BENZENE AND HEXAFLUOROBENZENE STUDIED BY RAMAN SPECTROSCOPY AND AB INITIO CALCULATIONS

Marcel Besnard [a], M. Isabel Cabaço [b,c], Yann Danten [a]

[a] *Institut des Sciences Moléculaires, CNRS (UMR 5255), Université Bordeaux 1, 351, Cours de la Libération 33405 Talence Cedex, France.*

[b] *Centro de Física Atómica da Universidade de Lisboa, Av. Prof. Gama Pinto 2, 1694-003 Lisboa, Portugal.*

[c] *Departamento de Física, Instituto Superior Técnico, UTL, Portugal.*

The polarized and depolarized Raman spectra of binary mixtures of carbon dioxide with benzene [1] or with hexafluorobenzene [2] have been measured along the isotherm 313 K as a function of CO_2 concentration (0.01 to 0.7 molar fractions in CO_2) by varying the pressure from 0.2 MPa to 6.2 MPa. Three main experimental features are detected and better observed in the mixtures with benzene. In the Raman forbidden region of the ν_2 bending mode of carbon dioxide, a new weak polarised band centred circa 655 cm^{-1} has been detected. The main perturbations of the Fermi dyad spectra of CO_2 have been assessed revealing in particular that each dyad component is constituted by two Lorentzian profiles. A new weak and polarised band has been detected between the components of the dyad.

These observations are rationalized on the ground of the results obtained in our previous experimental works (pure CO_2 [3] and CO_2-acetone mixtures [4]) and new ab-initio calculations have been performed predicting the formation of a hetero-dimer having a C_s symmetry for CO_2–C_6H_6 in which carbon dioxide is almost parallel to the ring plane. In contrast, for CO_2–C_6F_6 a C_{6v} structure with carbon dioxide perpendicular to the ring plane, i.e., along the main symmetry axis of C_6F_6 was predicted. We conclude that, on the short time scale and short spatial range probed by Raman spectroscopy, transient CO_2–C_6H_6 and CO_2–C_6F_6 hetero-dimers are put in evidence and that CO_2 exists within two environments. However, the experimental observations for CO_2–C_6F_6 show that the transient complex structure departs slightly from the predicted one. It is argued that it is this symmetry departure which is as the basis of the observation of the weak spectral features observed in the bending mode and Fermi dyad regions.

[1] Raman spectroscopy and ab initio investigations of transient complex formation in CO_2-benzene mixtures, M.Besnard, M.I.Cabaço, D.Talaga and Y. Danten, J. Chem. Phys. **2008**, *129*, 224511.
[2] Transient complex formation in CO_2-hexafluorobenzene mixtures: a combined Raman and ab initio investigation, M.Besnard, M.I.Cabaço and Y. Danten, J. Phys. Chem. A **2009**, *113*, 184.
[3] M. I. Cabaço, S. Longelin, Y. Danten, and M. Besnard, *J. Chem. Phys*. **2008**, *128*, 74507.

[4] M. Besnard, M. I. Cabaço, S. Longelin, T. Tassaing, and Y. Danten, *J. Phys. Chem. A* **2007**, *111*, 13371.

27. Marcel Besnard:, m.besnard@ism.u-bordeaux1.fr (Univ. Lisboa)
Study of the interactions of water diluted in imidazolium-based ionic liquids using vibrational spectroscopy and DFT calculations

M. Besnard[1], M. I. Cabaço[2] and Y. Danten[1]

[1] Institut des Sciences Moléculaires, CNRS (UMR 5255), Université Bordeaux, 351, Cours de la Libération 33405 Talence Cedex, France.
[2] Centro de Física Atómica da UL, Av. Prof. Gama Pinto 2, 1694-003 Lisboa Codex and Departamento de Física, Instituto Superior Técnico, UTL, Av. Rovisco Pais 1049-001 Lisboa, Portugal.

This study is aimed at providing physical insights about interactions of water diluted in imidazolium-based ionic liquids (ILs) using both DFT calculations and vibrational spectroscopy (IR absorption and Raman scattering). More precisely, we have investigated interactions of water with different cation-anion couples involving 1-butyl-3-methyl-imidazolium cations with a series of anions (namely, hexafluorophosphate (PF_6^-) and tetrafluoroborate (BF_4^-) tri-fluoro-methane-sulfonyl ($CF_3SO_3^-$) and bis-(tri-fluoro-methane-sulfonyl) imide $(CF_3SO_2)_2N^-$ anions).

The local organization in these water/ILs solutions have been assessed from the calculated structures of one water molecule interacting with a cation-anion pair dimer (at B3LYP/6-31+G** level). The predicted structures show that the water molecule preferentially interacts with two distinct anions by favoring symmetrical associations of type (A···H-O-H···A). We show the role of the non additive interactions between water and the ions by determining such associations and counterbalancing the primarily trend of water to form more directional hydrogen bonds.

The vibrational analysis shows that the doubly hydrogen-bonded nature of water interacting with the two anions engaged within the ion pair dimer leads to predict spectral features (band-centre positions, IR intensity values) which are found qualitatively in good agreement with the IR and Raman profiles measured in the region of the ν_1 and the ν_3 stretching modes of water (3400-3800 cm^{-1}). Thus, the local organization predicted from our DFT calculations appear quite representative of situations encountered at the 'molecular' level in real ILs solutions especially at low water concentrations (<0.1 mf.). Moreover, the appearance of a band in Raman associated with the ν_3 mode of 'monomeric' water/ILs solutions involving the PF_6^- and BF_4^- anions (not observed for H-bond interactions of water diluted in usual molecular solvents) suggests that the water molecule experiences a noticeable polarization effect due to the local electric field induced by surrounding ions. Thus, we emphasize that the water-anion interactions in the imidazolium ILs involve a more significant electrostatic character than that existing in the 'usual' H-bonding interactions of water in molecular systems

28. Reza M. Baram reza@cii.fc.ul.pt, (Univ. Lisboa)
Applications of space-filling packings

R. M. Baram, (in collaboration with P.G. Lind, J.S. Andrade Jr., H.J. Herrmann)

We describe an algorithm for randomly filling space with polydisperse discs fulfilling the particular condition of all discs being able to rotate simultaneously without sliding on each other at their contact points. Two applications of such packings, which we call bearings, are given.
The first one addresses geometrical models for seismic gaps: we show that space-filling packing are able to reproduce the size distributions observed in recent studies of real fault gouges, namely their range of values in the spectrum of fractal dimensions observed along real faults. This finding strengthen the evidence that polydisperse bearings may explain the occurrence of seismic gaps in nature.
The second application deals with the study drag-induced diffusion of massive particles in scale-free velocity fields. Here, each rotating disc is taken as a vortex within a fluid and has a linear velocity profile inside. In this way, we obtain a velocity field containing eddies of many different scales.