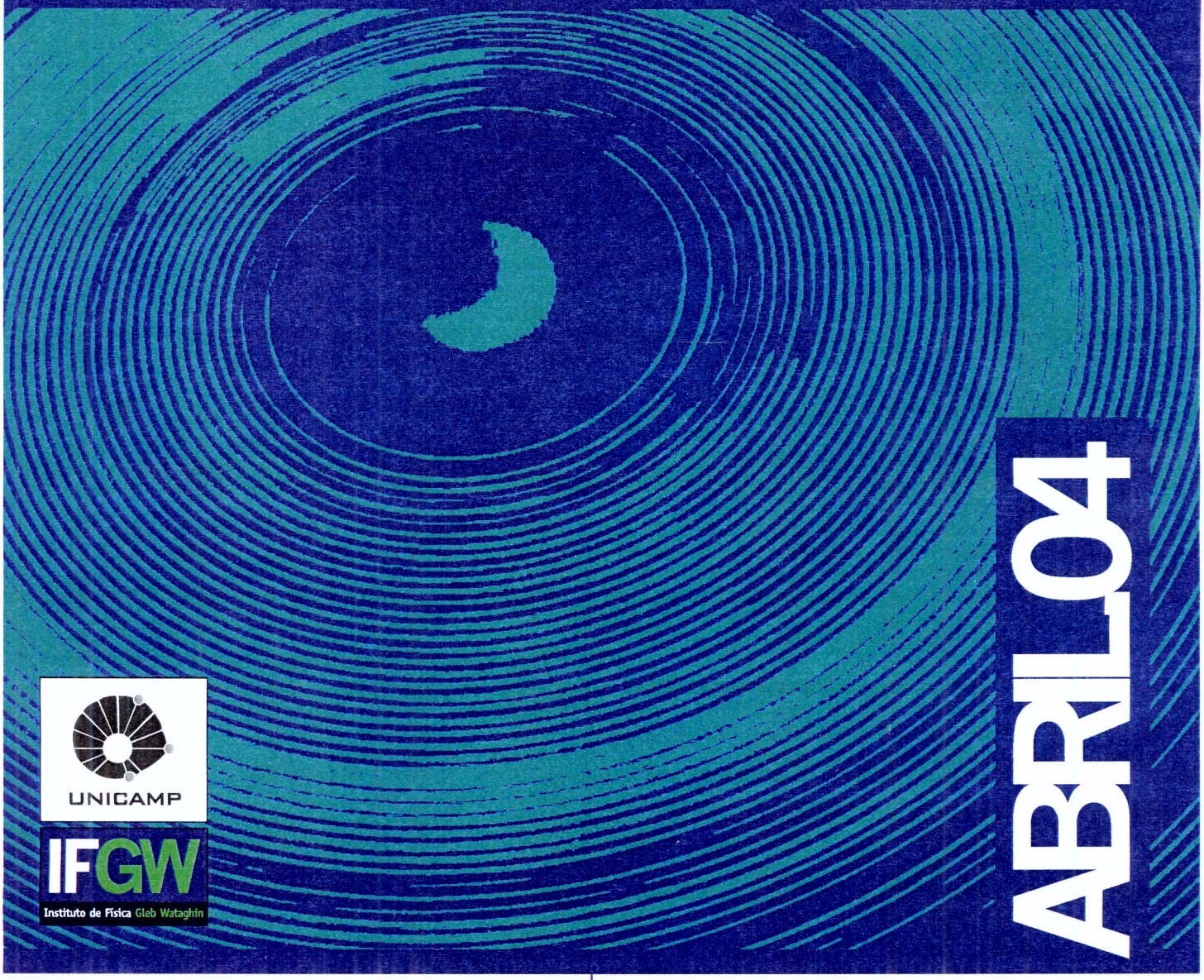
Abstracta

Ano V I- N.02



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TRABALHOS ACEITOS PARA PUBLICAÇÃO

A 001- 04 Electronic excitation of N2 by positron impact.

A 002- 04 Positron impact electronic excitation of N2.

A 003 -04 Electron-impact excitation of H2: Minimal Orbital Basis for Single Configuration Interaction.

A 004 - 04 Mechanical properties of nanosprings.

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A 007 -04 Characteization of Nanometric Quantum Wells in Semiconductor Heteostructures by Optical Spectroscopy.

A 008 - 04 The Structure and Dynamics of Carbon Nanoscrolls.

A 009- 04 Strong spatial beryllium doping selectivity on InGaP layers grown on pre-patterned GaAs substrates by Chemical Beam Epitaxy.

A 010- 04 Heat capacity studies of Ce and Rh site substitution in the heavy-fermion antiferromagnet CeRhIn5: Short-range magnetic interactions and non-Fermi-liquid behavior.

A 011- 04 Magnetic structure of CeRhIn5 as a function of pressure and temperature

A 012- 04 EMERGENCE OF ALLOMETRIC SCALING IN GENEALOGICAL TREES.

A 013 - 04 MUTATIONAL EFFECTS ON THE CLONAL INTERFERENCE PHENOMENON.

A 014- 04 Dynamics of fixation of advantageous mutations.

TRABALHOS PUBLICADOS

P 031 - 04 À P 052- 04

TRABALHOS ACEITOS PARA PUBLICAÇÃO

A 001- 04 Electronic excitation of N2 by positron impact.

Puspitapallab Chaudhuri,Marcio T. do N. Varella, Claudia R. C. de Carvalho and Marco A. P. Lima

We present cross sections of electronic excitation of nitrogen molecule (N2) by positron impact using the Schwinger multichannel method (SMC). Our calculated cross sections are compared with the recent and the only available experimental data of Sullivan *et al.* (J. P. Sullivan, J. P. Marler,S. J. Gilbert, S. J. Buckman and C. M. Surko, Phys. Rev. Lett. 87 073201-1 (2001)). Present theoretical results for excitation to the $a1\,g$ states do not reproduce the near{threshold structure observed in the experimental data.

Physical Review A, accepted on February 2004.

A 002- 04 Positron impact electronic excitation of N2.

Puspitapallab Chaudhuri, Marcio T. do N. Varella, Claudia R. C. de Carvalho and Marco A. P. Lima

We present the results of scattering cross sections for positron impact excitation of electronic states of Nitrogen molecule (N2) using the Schwinger multichannel method (SMC). All calculated cross sections took three collision channels into account ($X1\,g$ and degenerate $a1\,g$ states). Present theoretical results for excitation to the $a1\,g$ states failed to reproduce the near{threshold structure observed in the recent and the only available experimental data [Sullivan *et al.*, Phys.Rev. Lett. 87 073201-1 (2001)]. Scattering calculations from the $a1\,g$ states (elastic and superelastic) are also reported. A spurious resonant structure found in the excitation to the $a1\,g$ states was detected in a square integrable basis set calculation designed to reproduce the ¯rst Born approximation (FBA). Such spurious structure was removed by taking out the trial con¯guration state functions in which the positron was weakly coupled to the target. This may be a promising technique to separate unphysical resonances from the physical ones. We also observe that a combination between SMC scattering amplitudes ($l \cdot 2$) with FBA ones ($l \ , \ 3$) signi¯cantly improved the cross sections at higher energies.

Nuclear Instruments and Method B, accepted on March 2004.

A 003 -04 Electron-impact excitation of H2: Minimal OrbitalBasis for Single Configuration Interaction.

Romarly F da Costa, Fernando J da Paixao, and Marco A P Lima

We report theoretical di®erential excitation cross sections for scattering of electrons by H2 molecules using the Schwinger Multichannel Approach (SMC). This study di®ers from previous applications of the SMC method in the description of the excited states (which are now obtained through single con¯guration interaction technique) and in the level of the multichannel coupling. The calculation is performed with singlet and triplet states present in the manifold. The results given by this strategy show a signi¯cant improvementtowards experimental data in comparison with earlier two-state close coupling calculations.

Journal of Physics B, accepted on March 2004.

A 004 - 04 Mechanical properties of nanosprings.

Alexandre F. da Fonseca and Douglas S. Galvão

Nanostructures (nanotubes, nanowires, etc.) have been object of intense theoretical and experimental investigations in the last years. Among these structures helical nanosprings or nanocoils have attracted particular interest due to their special mechanical properties. In this work we investigate structural properties of nanosprings in the Kirchoff rod model. We derived expressions that can be used experimentally to obtain nanosprings Young's modulus and Poisson's ratio values. Our results also might explain why the presence of catalytic particles is so important in nanostructure growths.

Physical Review Letters, accepted on March 2004

A 005- 04 Electron collisions with isomers of C4H8 and C4H10.

A R Lopes1, M H F Bettega1, M A P Lima2 and L G Ferreira2

We report integral, differential and momentum transfer cross sections for elastic scattering of low-energy electrons by several isomers of the C4H8 molecules, such as isobutene, trans-2-butene, cis-2-butene, skew-1-butene and syn-1-butene, and by two isomers of C4H10, the isobutane and the butane molecules. To calculate the cross sections, we use the Schwinger multichannel method with pseudopotentials (Bettega *et al* 1993 *Phys. Rev.* A **47** 1111) applied at the static exchange level of approximation for incident energies from 10 to 50 eV. Although the C4H8 isomers have different geometric structures, our results show that the integral cross sections for each of these isomers present a broad shape resonance around 10 eV; our results also show that for all C4H8 molecular targets, integral cross sections are very similar in shape and magnitude. Similarities are also found in the momentum transfer and in the differential cross sections of these isomers. The same pattern is found in the cross sections of the C4H10 isomers. Through comparison of the integral and momentum transfer cross sections of 1,3-butadiene (C4H6), trans-2-butene (C4H8) and butane (C4H10), all belonging to the C2h group and having similar structures, we discuss the role of the hydrogen atoms in the scattering process by these molecules. Further we show that the integral elastic cross sections of all simple hydrocarbons present strong similarities after a scaling. We present a simple geometric model for this scaling that works quite well for a whole family of C*n*H*m* molecules (with combinations of n = 1, 2, 3, 4 and m = 2, 4, 6, 8, 10).

Journal of Physics B., accepted on March 2004.

A 006- 04 Low Energy Positron Scattering by SF6 and CO2.

S. d'A. Sanchez´, F. Arretche, M. T. do N. Varella and M. A. P. Lima

In this work we present theoretical integral (ICS) and differential (DCS) cross section calculations for low-energy positron scattering by SF6 and CO2 molecules. Our scattering wave functions were obtained with the Schwinger Multichannel Method (SMC) [6] at the static and static-plus-polarization levels of approximation. The elastic DCS were calculated over an energy interval ranging from 4 eV up to 50 eV for SF6 and from 1 eV up to 20 eV for CO2: The results show, in general, good agreement with recent experimental data [8]. We found a Ramsauer-Townsend minimum in eþ ^ CO2 calculations, even though no signature of virtual state formation was observed, contrasting with the well-known case of electron scattering [17].

Physica Scripta, accepted on March 2004

A 007 -04 Characteization of Nanometric Quantum Wells in Semiconductor Heteostructures by Optical Spectroscopy.

E. Laureto, A. R. Vasconcellos, E. A. Meneses, R. Luzzi

Growth of heterostructures produces quantum wells with fractal-like interfaces which greatly affect their optical and transport properties.A systematic study of growth followed by realization of optical experiments was performed. The spectra obtained show some kind of " anomalies" depending on the growth characteristics. They are analized resorting to an unconventional statistical mechanics which allows to correlate growth conditions and surface roughness and their influence on the experimental result, allowing to obtain a picture of the physics of the phenomenon.

International journal of Modern physics B, accepted on march 2004.

A 008 - 04 The Structure and Dynamics of Carbon Nanoscrolls.

Scheila. F. Braga, Vitor. R. Coluci, Sergio. B. Legoas, Ronaldo Giro, Douglas. S. Galvão, and Ray. H. Baughman

Carbon nanotube scrolls (CNSs) provide an interesting form of carbon that ideally consists of a single sheet of graphite that is spiral wrapped to form a nanotube. We here use molecular dynamics simulations to investigate CNS formation, stability, and the structural effects due to charge injection. CNS formation is seen to automatically occur when a critical overlap between sheet layers is achieved for the partially curled sheet. We observed that charge injection causes unwinding of the CNSs, which might be important for the application of CNSs as nano-mechanical actuators.

Nano Letters, accepted on March 2004

A 009- 04 Strong spatial beryllium doping selectivity on InGaP layers grown on pre-patterned GaAs substrates by Chemical Beam Epitaxy.

M. P. P. de Castro, A. A. Vonzuben, and N. C.Frateschi*, L.L.E. Santo, D. S. Galvão, J. Bettini and M. M. G. de Carvalho

We present an investigation of beryllium doping selectivity in InGaP layers grown by Chemical Beam Epitaxy (CBE) on pre-patterned substrates. We observed a resistivity of 3.1x10-2 Wcm and 4.5x10-2 Wcm for (111)A planes with the growth at 500 0C and 540 0C, respectively. The layers on (001) planes show a resistivity of 8.9x10-1 Wcm with the growth at 500 0C, being essentially undoped with the growth at 540 0C . We show how this strong doping selectivity can be explained by Be3P2 cluster formation growth, which depends on growth temperature and planar crystalline structure.

Journal of Crystal Growth, accepted on March 2004.

A 010- 04 Heat capacity studies of Ce and Rh site substitution in the heavy-fermion antiferromagnet CeRhIn5: Short-range magnetic interactions and non-Fermi-liquid behavior.

Light BE, Kumar RS, Cornelius AL, Pagliuso PG, Sarrao JL

In heavy fermion materials superconductivity tends to appear when long-range magnetic order is suppressed by chemical doping or applying pressure. Here we report heat capacity measurements on diluted alloys of the heavy fermion superconductor CeRhIn5. Heat capacity measurements have been performed on CeRh1-yIryIn5 (yless than or equal to0.10) and Ce1-xLaxRhIn5 (xless than or equal to0.50) in applied fields up to 90 kOe to study the effect of doping and magnetic field on the magnetic ground state. The magnetic phase diagram of CeRh0.9Ir0.1In5 is consistent with the magnetic structure of CeRhIn5 being unchanged by Ir doping. Doping of Ir in small concentrations is shown to slightly increase the antiferromagnetic transition temperature T-N (T-N=3.8 K in the undoped sample). La doping which causes disorder on the Ce sublattice is shown to lower T-N with no long-range order observed above 0.34 K for Ce0.50La0.50RhIn5. Measurements on Ce0.50La0.50RhIn5 show a coexistence of short-range magnetic order and non-Fermi-liquid behavior. This dual nature of the Ce 4f electrons is very similar to the observed results on CeRhIn5 when long-range magnetic order is suppressed at high pressure.

Physical Review B 69[024419] Jan 2004.

A 011- 04 Magnetic structure of CeRhIn5 as a function of pressure and temperature

Llobet A, Gardner JS, Moshopoulou EG, Mignot JM, Nicklas M, Bao W, Moreno NO, Pagliuso PG, Goncharenko IN, Sarrao JL, Thompson JD

We report magnetic neutron-diffraction and electrical resistivity studies on single crystals of the heavy-fermion antiferromagnet CeRhIn5 at pressures up to 2.3 GPa. These experiments show that the staggered moment of Ce and the incommensurate magnetic structure change weakly with applied pressure up to 1.63 GPa, where resistivity, specific heat and nuclear quadrupole resonance measurements confirm the presence of bulk superconductivity. This work places important constraints on an interpretation of the relationship between antiferromagnetism and unconventional superconductivity in CeRhIn5.

PHYSICAL REVIEW B 69 (2): Art. No. 024403 JAN 2004

A 012- 04 EMERGENCE OF ALLOMETRIC SCALING IN GENEALOGICAL TREES.

PAULO R. A. CAMPOS, and VIVIANE M. DE OLIVEIRA
LEONARDO P. MAIA

We investigate the emergence of power-law scalings in genealogical trees. Especially, we study the topological properties of genealogical trees both in the neutral evolution and the selective evolution. In all instances, we observe that the topologies of these trees are well described by a power-law scaling $C_k \sim A_k^{\eta}$ **where** A_k is the number of nodes which are direct or indirect descendants of node k and $C_k = \Sigma_j A_j$ where the sum istaken over all nodes that contribute to A_k. This relation is well known in transportationnetworks as well as in metabolic networks, and it is referred to as allometric scaling.Furthermore, we observe a slight dependence of the scaling exponent □ on the intensity of selection.

Advances in Complex Systems, accepted on March 2004.

A 013 - 04 MUTATIONAL EFFECTS ON THE CLONAL INTERFERENCE PHENOMENON.

PAULO R. A. CAMPOS AND VIVIANE M. DE OLIVEIRA

We study the process of fixation of beneficial mutations in an asexual population by means of a theoretical model. Particularly, we wish to investigate how the supply of deleterious and beneficial mutations influences the dynamics of the adaptive process of an evolving population. It is well known that the deleterious mutations drastically affect the fate of beneficial mutations. In addition, an increasing supply of favorable mutations, to compensate the decay of the fitness due to the accumulation of deleterious mutations, produces the clonal interference phenomenon where advantageous mutations in distinct lineages compete to reach fixation. This competition imposes a limit to the speed of adaptation of the population. Intuitively, we would expect that the interplay of the two mechanisms would conspire to ensure fixation of only large-effect beneficial mutations. Our results, however, show that beneficial mutations of small effect have an increased probability of fixation when both beneficial and deleterious mutations rates are increased.

EVOLUTION accepted on March 2004.

A 014- 04 Dynamics of fixation of advantageous mutations.

Viviane M. de Oliveira, Paulo R.A. Campos*

We investigate the process of fixation of advantageous mutations in an asexual population. We assume that the effect of each beneficial mutation is exponentially distributed with mean value $\varpi_{med} = 1/\beta$. The model also considers that the effect of each new deleterious mutation reduces the fitness of the organism independent on the previous number of mutations. We use the branching process formulation and also extensive simulations to study the model. The agreement between the analytical predictions and the simulational data is quite satisfactory. Surprisingly, we observe that the dependence of the probability of fixation P_{fix} on the parameter ϖ_{med} is precisely described by a power-law relation, $P_{fix} \sim \varpi^{\gamma}_{med}$. The exponent γ is an increasing function of the rate of deleterious mutations U, whereas the probability P_{fix} is a decreasing function of U. The mean value ϖ_{fix} of the beneficial mutations which reach ultimate fixation depends on U and ϖ_{med}. The ratio $\varpi_{fix}/\varpi_{med}$ increases as we consider higher values of mutation value U in the region of intermediate to large values of ϖ_{med}, whereas for low ϖ_{med} we observe the opposite behavior.

Physica A, accepted on March 2004

Trabalhos Publicados

MARÇO/ABRIL 2004

P 031- 04 "Atmospheric neutrinos: LMA oscillations, U e3 induced interference and CP-violation".

Peres, O. L. G. and Smirnov, A. Y.

We consider oscillations of the low energy (sub-GeV sample) atmospheric neutrinos in the three neutrino context. We present the semi-analytic study of the neutrino evolution and calculate characteristics of the e-like events (total number, energy spectra and zenith angle distributions) in the presence of oscillations. At low energies there are three different contributions to the number of events: the LMA contribution (from nu(e)-oscillations driven by the solar oscillation parameters), the U-e3-contribution proportional to s(13)(2), and the U-e3-induced interference of the two amplitudes driven by the solar oscillation parameters. The interference term is sensitive to the CP-violation phase. We describe in details properties of these contributions. We find that the LMA, the interference and U-e3 contributions can reach 5-6%, 2-3% and 1-2% correspondingly. An existence of the significant (> 3-5%) excess of the e-like events in the sub-GeV sample and the absence of the excess in the multi-GeV range testifies for deviation of the 2-3 mixing from maximum. We consider a possibility to measure the deviation as well as the CP-violation phase in future atmospheric neutrino studies. (C) 2004 Elsevier B.V. All rights reserved.

Nuclear Physics B 680[1-3], 479-509. 2004.

P 032- 04 "Cold electrode erosion model for pulsed arcs applied to the electrical discharge machining process".

Sharakhovsky, L. I., Marotta, A., and Essiptchouk, A. M

A simple erosion model for electrical discharge machining (EDM) is proposed and compared to other authors' cathode experimental data. From these comparisons, the effective arc spot current density and erosion enthalpy have been obtained. The good agreement between the experimental results and the theoretically calculated erosion curve validates the model.

High Temperature Material Processes 7[3], 407-413. 2003.

P 033- 04 "Comprehensive spectroscopic study of nitrogenated carbon nanotubes".

Droppa, R., Ribeiro, C. T. M., Zanatta, A. R., dos Santos, M. C., and Alvarez, F.

Carbon nanotubes with different nitrogen contents were produced by the arc-discharge technique. The samples were first submitted to a concentration process (purification) and analyzed by x-ray photoelectron spectroscopy, electron-energy-loss spectroscopy, electron transmission, and scanning electron microscopy to study the materials structure and morphology. Measured values of nitrogen concentration were below 5 at. % and varied with the nitrogen partial pressure inside the arc-discharge chamber. Using an optical microscope, highly localized regions of the samples (similar to1 mm(2)) were irradiated by an Ar ion laser. Controlling the laser intensity, further local purification was induced and information about the evolution of the structural order of the nanotube samples with different contents of nitrogen was obtained.

Physical Review B 69[4]. 2004.

034- 04 "Diamond-like carbon coatings on Ti-13Nb-13Zr alloy produced by plasma immersion for orthopaedic applications".

Uzumaki, E. T., Lambert, C. S., and Zavaglia, C. A. C.

Diamond-like carbon (DLC) films have been intensively studied with a view to improving orthopaedic implants. Various techniques have been employed to manufacture DLC films, and recently, the plasma immersion process has been used to provide non-line-of-sight deposition on three-dimensional pieces with complex shapes. In this method, the whole surface of the target is coated, even without moving the sample, and without an intermediate layer. DLC films were deposited on a silicon wafer and Ti-13Nb-13Zr alloy substrates, using the plasma immersion process. The films were analysed by Raman spectroscopy, atomic force microscopy (AFM), and nanoindentation. As examples, uniformly DLC coated orthopaedic implants (knee implant and femoral head) are shown.

Bioceramics, Vol 16 254-2, 435-437. 2004.

P 035- 04 "Elastic and absorption cross sections for electron scattering by ethylene in the intermediate energy range".

Brescansin, L. M., Rawat, P., Iga, I., Homem, M. G. P., Lee, M. T., and Machado, L. E.

In this work, we present a joint theoretical and experimental study on electron scattering by C2H4 in the intermediate energy range. Calculated elastic differential, integral, and momentum-transfer as well as total (elastic + inelastic) and absorption cross sections are reported at impact energies ranging from 10 to 500 eV. Also, experimental absolute elastic cross sections are reported in the 100-500 eV range. The measurements were performed using a crossed electron beam-molecular beam geometry. The angular distributions of the scattered electrons were converted to absolute cross sections using the relative flow technique. Theoretically, a complex optical potential was used to represent the electron-molecule interaction dynamics. The Schwinger variational iterative method combined with the distorted-wave approximation was used to solve the scattering equations. The comparison between our calculated and measured results, as well as with other experimental and theoretical data available in the literature, is encouraging.

Journal of Physics B-Atomic Molecular and Optical Physics 37[2], 471-483. 2004.

P 036- 04 "Hidden scaling in the quantum Hall metal-insulator transition".

Moriconi, L., Pereira, A. L. C., and Schulz, P. A.

Scaling properties of the quantum Hall metal-insulator transition are severely affected by finite-size effects in small systems. Surprisingly, despite the narrow spatial range where probability structure functions exhibit multifractal scaling, we clearly verify the existence of extended self-similarity-a hidden infrared scaling phenomenon related to the peculiar form of the crossover at the onset of nonmultifractal behavior. As finite-size effects get stronger for structure functions with negative orders, the parabolic approximation for the multifractal spectrum loses accuracy. However, by means of an extended self-similarity analysis, an improved evaluation of the multifractal exponents is attained for negative orders too, rendering them consistent with previous results, which rely on computations performed for considerably larger systems.

Physical Review B 69[4]. 2004.

P 037- 04 "Hybrid materials derived from divinylbenzene and cyclic siloxane".

Pinho, R. O., Radovanovic, E., Torriani, I. L., and Yoshida, I. V. P.

In this work, hybrid materials were synthesized as self-supported films from divinylbenzene and cyclic siloxane, in different compositions, by hydrosilylation reaction. These films showed good thermal and mechanical properties. Their glass transition temperatures were higher than those of conventional silicone networks, and dependent on divinylbenzene amounts. Films were homogeneous and no pores were observed by field emission electron scanning microscopy. Relationships between surface roughness and composition of the obtained films were discussed. The nanomorphology of the materials was studied by small angle X-ray scattering, showing polydispersed nano-sized heterogeneities. The gas permeability of the hybrid films was investigated, and the results suggested low permeable behaviour to gases, but high ideal selectivities to some pairs of gases, such as H-2/O-2.

European Polymer Journal 40[3], 615-622. 2004.

P 038- 04 "Infrared optoacoustic spectroscopy of CHD2OH around 10R and 10P CO2 laser lines".

Viscovini, R. C., Cruz, F. C., Scalabrin, A., and Pereira, D.

In this work we present results of an investigation on Doppler limited infrared absorbing transitions of CHD2OH by optoacoustic detection. It is an alternative and attractive technique to be applied to this methanol isotopomer, in comparison to Fourier transform spectroscopy. Using a waveguide CO2 laser of 290 MHz tunability on each line, we were able to observe 60 IR absorptions, most of them of large offset. The data will be useful in the theoretical analysis of this molecule, as well as in the generation of far-infrared (FIR) laser radiation in optically pumped molecular lasers

International Journal of Infrared and Millimeter Waves 25[2],257-275. 2004.

P 039- 04 "Low-energy electron collisions with C4H6 isomers".

Lopes, A. R., Lima, M. A. P., Ferreira, L. G., and Bettega, M. H. F.

We report integral, differential, and momentum-transfer cross sections for elastic scattering of low-energy electrons by C4H6 isomers, namely, 1,3-butadiene, 2-butyne, and cyclobutene. We use the Schwinger multichannel method with pseudopotentials [M. H. F. Bettega, L. G. Ferreira, and M. A. P. Lima, Phys. Rev. A-47, 1111 (1993)] at the static-exchange approximation to compute the cross sections for energies from 10 to 60 eV. In particular, we discuss the isomer effect, reported by experimental studies for isomers Of C3H4 and C4H6. We also calculate the total ionization cross section using the binary-encounter-Bethe model for 2-butyne and 1,3-butadiene, and estimate the inelastic cross section for these two isomers.

Physical Review A 69[1]. 2004.

P 040- 04 "Lower bounds on the entanglement of formation for general Gaussian states".

Rigolin, G. and Escobar, C. O.

We derive two lower bounds on entanglement of formation for arbitrary mixed Gaussian states by two distinct methods. To achieve the first one we use a local measurement procedure that symmetrizes a general Gaussian state and the fact that entanglement cannot increase under local operations and classical communications. The second one is obtained via a generalization to mixed states of an interesting result already known for pure states, which says that squeezed states are those that, for a fixed amount of entanglement, maximize Einstein-Podolsky-Rosen-like correlations.

Physical Review A 69[1]. 2004.

P 041- 04 "Molecular dynamics simulations of C-60 nanobearings".

Legoas, S. B., Giro, R., and Galvao, D. S.

Recently was reported an ultra-lubricated system based on C-60 molecules deposited over graphite layers. In that work a stick-slip rolling model for C-60 molecules was proposed to explain the observed ultra-low friction force. In this Letter, we report the first molecular dynamics studies for these systems. Our results show that the AB stacking is not observed and the main experimental features can be explained without invoking stick-slip motions. (C) 2004 Elsevier B.V. All rights reserved.

Chemical Physics Letters 386[4-6], 425-429. 2004.

P 042-04 "Nanocomposites of amorphous hydrogenated carbon and siloxane networks produced by PECVD".

Trasferetti, B. C., Gelamo, R. V., Rouxinol, F. P., de Moraes, M. A. B.,Goncalves, M. D., and Davanzo, C.

Chemistry of Materials 16[4], 567-569. 2004.

P 043- 04 "Observation of multipolar scattering in holmium with non-resonant X-ray scattering at the LNLS".

Yokaichiya, F. and Giles, C.

Multipolar ordering in metallic holmium 4f shell was studied by non resonant X-ray scattering at the helical antiferromagnetic phase. The quadrupolar nature of the 2tau satellite peaks is confirmed from the good agreement of the measured values of the form factor with calculated values for quadrupolar scattering. The strong spin-orbit coupling drives the multipolar order, experimentally confirmed through the temperature dependence of the quadrupolar ordering wave vector 2tau. Form factors of the satellite peaks observed at 4tau are higher than those expected for the octupolar scattering. (C) 2003 Elsevier B.V. All rights reserved.

Physica B-Condensed Matter 345[1-4], 82-85. 2004.

P 044- 04 "Phonon activity and intermediate glassy phase of YVO3".

Massa, N. E., Piamonteze, C., Tolentino, H. C. N., Alonso, J. A., Martinez-Lope, M. J., and Casais, M. T.

We show that in YVO3 additional hard phonons gradually become zone center infrared active below similar to210 K, verifying that a lattice phase transition takes place at about that temperature. Their gradual increment in intensity between similar to210 and similar to77 K is associated with a "glassy" behavior found in the temperature-dependent V K edge pseudoradial distribution. This translates into an increase in the Debye-Waller factors ascribed to the appearance of V local structural disorder below similar to150 K. Conflicts between various ordering mechanisms in YVO3 bring up similarities of the intermediate phase to known results in dielectric incommensurate systems, suggesting the formation of commensurate domains below 116 K, the onset temperature of G-type antiferromagnetism. We propose that similar to210 and similar to77 K be understood as the temperatures where the commensurate-incommensurate and incommensurate-commensurate "lock-in" phase transitions take place. We found support for this interpretation in the inverted lambda shapes of the measured heat capacity and in the overall temperature dependence of the hard phonons.

Physical Review B 69[5]. 2004.

P 045- 04 "Preparation and characterization of new niobophosphate glasses in the Li2O-Nb2O5-CaOP2O5 system".

Mazali, I. O., Barbosa, L. C., and Alves, O. L.

In the present work we describe the synthesis, spectroscopy, thermal and chemical durability properties of the vitreous system Li2O-Nb2O5-CaO-P2O5 (LNCP). Investigations of the short-range order by Fourier transform infrared, Raman, UV-VIS and P-31 MAS-NMR spectroscopies suggest that the network former glass consists of Nb octahedra linked to pyro/orthophosphate units through Nb-O-P bonds. The presence of modifier cations (Li+ and Ca2+) promotes depolymerization of the P-O-P chains, yielding pyro/orthophosphate units. The presence of this kind of structure accounts for the improvement of the chemical durability at low pH when the Nb content in the LNCP glass composition is high. The density and linear refractive indices of LNCP glasses increased linearly as the Nb2O5/P2O5 molar ratio increased, as a consequence of P2O5 substitution by Nb2O5 as the glassformer. The dependence of the glass transition temperature, the softening temperature and the crystallization temperature on the Nb2O5/P2O5 ratio exhibits the same behavior. On the other hand, the thermal expansion coefficient decreases with the increased Nb2O5/P2O5 ratio. (C) 2004 Kluwer Academic Publishers.

Journal of Materials Science 39[6], 1987-1995. 2004.

P 046- 04 "Quintessential inflation and non-oscillatory reheating model".

Campos, A. H., Reis, H. C., and Rosenfeld, R

A numerical study of the non-oscillatory reheating mechanism in a quintessential inflation context shows that high reheating temperature can be achieved compared with the usual reheating mechanism in which particles are produced gravitationally. We find that even for a very small coupling between the inflaton field and a massless scalar field, the non-oscillatory reheating production of particles dominates over the gravitational production mechanism.

Nuclear Physics B-Proceedings Supplements 127, 133-137. 2004.

P 047- 04 "Rapid method for evaluating reversed-phase high performance liquid chromatography column stability".

Fonseca, D. A., Gutierrez, H. R., Collins, K. E., and Collins, C. H.

A procedure is presented for the rapid evaluation of HPLC stationary phase stability at pH 8.4 or 10.1 using a temperature of 60degreesC. Mobile phase (MeOH-0.1 mol 1(-1) aqueous NaHCO3, 50:50, v/v) is continuously passed through the column with periodic injections of a test solution until the several chromatographic parameters of the resulting chromatograms are degraded. The tests were applied to several commercial and laboratory-made stationary phases. After degradation two of these phases, one commercial and one laboratory-made, were examined by elemental analysis and scanning electron microscopy to elucidate the degradation process. (C) 2004 Elsevier B.V. All rights reserved

Journal of Chromatography A 1030[1-2], 149-155. 2004.

P 048- 04 "Stark effects on Coulomb-bound states in GaAs (Ga,Al)As quantum wells: virial theorem and scaling properties".

Reyes-Gomez, E., Villalba-Chavez, S., Oliveira, L. E., and Dios Leyva,M.

The effects of applied electric fields on donor and exciton states confined in GaAs-(Ga,Al)As quantum wells are studied in the effective mass approximation and within the variational and fractional-dimensional space approaches. In the fractional-dimensional scheme, an effective isotropic medium is used to model the anisotropic Coulomb-bound state + quantum well + electric-field system, whereas a hydrogenic-like wave function is used in the variational procedure. Results are obtained for the binding energies, virial-theorem values, and scaling properties of the Coulomb-bound states under growth-direction applied electric fields. We show that a ground-state wave function assumed as a D-dimensional hydrogenic wave function leads to a virial-theorem value of 2 and a hyperbolic scaling for binding energies of Coulomb-bound states versus quantum-confined Bohr radii, in contrast with results using the variational approach. Both methods result in Stark shifts for the exciton-peak energies in good agreement with electroabsorption experiments.

Journal of Physics D-Applied Physics 37[5], 660-667. 2004.

P 049- 04 "Spurious four-wave mixing in two-pump fiber optic parametric amplifiers".

Callegari, F. A., Boggio, J. M. C., and Fragnito, H. L.

We present an experimental study on four-wave mixing (FWM) between two signals within a two-pump fiber-optical parametric amplifier (2P-FOPA). We demonstrate that the intensity of FWM spurious tones depend strongly on the signal power and length of the nonlinear medium and present two regimes as a function of the pumps' power. We also compare the amounts of FWM as a function of channel spacing in the 2P-FOPA with or without pumps and show that the presence of parametric gain enhances FWM over a broad spectral range.

Ieee Photonics Technology Letters 16[2], 434-436. 2004.

P 050- 04 "The Brazilian spherical detector: progress and plans".

Aguiar, O. D., Andrade, L. A., Barroso, J. J., Camargo, L., Carneiro, L. A., Castro, C. S., Castro, P. J., Costa, C. A., Costa, K. M. F., de Araujo, J. C. N., de Lucena, A. U., de Paula, W., Neto, E. C. D., de Souza, S. T., Fauth, A. C., Frajuca, C., Frossati, G., Furtado, S. R., Lima, L. C., Magalhaes, N. S., Marinho, R. M., Matos, E. S., Melo, J. L., Miranda, O. D., Oliveira, N. F., Paleo, B. W., Remy, M., Ribeiro, K. L., Stellati, C., Velloso, W. F., and Weber, J.

We are building the Schenberg gravitational wave detector at the Physics Institute of the University of Sao Paulo as programmed by the Brazilian Graviton Project. The antenna and its vibration isolation system are already built, and we have made a first cryogenic run for an overall test, in which we measured the antenna mechanical Q (figure of merit). We also have built a 10.21 GHz oscillator with phase noise performance better than -120 dBc at 3.2 kHz to pump an initial CuA16% two-mode transducer. We plan to prepare this spherical antenna for a first operational run at 4.2 K with a single transducer and an initial target sensitivity of h similar to 2 x 10(-21) Hz(-1/2) in a 50 Hz bandwidth around 3.2 kHz soon. Here we present details of this plan and some recent results of the development of this project

***Classical and Quantum Gravity* 21[5], S457-S463. 2004.**

P 051- 04 "The ion exchange properties and equilibrium constants of Li+, Na+ and K+ on zirconium phosphate highly dispersed on a cellulose acetate fibers surface".

Borgo, C. A., Lazarin, A. M., Kholin, Y. V., Landers, R., and Gushikem, Y.

Highly dispersed zirconium phosphate was prepared by reacting celullose acetate/ZrO2 (ZrO2 = 11 wt%, 1.0 mmol g(-1) of zirconium atom per gram of the material) with phosphoric acid. High power decoupling magic angle spinning (HPDEC-MAS) P-31 NMR and X-ray photoelectron spectroscopy data indicated that HPO42- is the species present on the membrane surface. The specific concentration of acidic centers, determined by ammonia gas adsorption, is 0.60 mmol g(-1). The ion exchange capacities for Li+, Na+ and K+ ions were determined from ion exchange isotherms at 298 K and showed the following values (in mmol g(-1)): Li+= 0.05, Na+= 0.38 and K+= 0.57. Due to the strong cooperative effect, the H+/ Na+ and H+/ K+ ion exchange is of non ideal nature. These ion exchange equilibria were treated with the use of models of fixed tridentate centers, which consider the surface of the sorbent as polyfunctional sorption centers. Both the observed ion exchange capacities with respect to the alkaline metal ions and the equilibrium constants are discussed by taking into consideration the sequence of the ionic hydration radii for Li+, Na+ and K+. The matrix affinity for the ions decreases with increasing the cations hydration radii from K+ to Li+. The high values of the separation factors SNa+/Li+ and SK+/Li+ (up to several hundreds) support the application of this material for the quantitative separation of Na+ and K+ from Li+ from a mixture containing these three ions.

Journal of the Brazilian Chemical Society 15[1], 50-57. 2004.

P 052- 04 "Total elastic cross section for (H)over-bar-H scattering at thermal energies".

Sinha, P. K., Chaudhuri, P., and Ghosh, A. S.

This paper reports the elastic scattering cross sections for a few low-lying partial waves and also the converged elastic cross sections with added partial waves in the energy range 10(-10)-10(-2) a.u. for the (H) over bar -H system using atomic orbital techniques. The present s-wave predictions are in good agreement with the other existing theoretical estimates. Nonzero low-order partial-wave elastic cross sections show dips like for s-wave scattering. The, converged elastic cross section shows structurelike behavior in the energy range 4.2 X 10(-4)-10(-2) a.u

Physical Review A 69[1]. 2004.

Abstracta

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