Abstracta

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TRABALHOS ACEITOS PARA PUBLICAÇÃO

A 015 -04 Anisotropic Manifestation of Short-range Magnetic Correlations in $Ce_{0.6}La_{0.4}RhIn_5$.

A 016- 04 Anomalous *f*-electron Hall Effect in the Heavy-Fermion System $CeTIn_5$ (T = Co, Ir, or Rh).

A 017 - 04 "Origin of the A_{1g} Electronic Raman Scattering Peaks in the Superconducting State of $YBa_2Cu_3O_{7-}$d.

A 018-04 Rare earth doped silicon nanocrystals derived from an erbium amidinateprecursor.

L 001- 04 Ensemble formalisms for nonequilibrium systems and an associated irreversible statistical thermodynamics .

TRABALHOS PUBLICADOS

P 053 - 04 À P 096- 04

TRABALHOS ACEITOS PARA PUBLICAÇÃO EM PERIÓDICOS

A 015 -04 Anisotropic Manifestation of Short-range Magnetic Correlations in $Ce_{0.6}La_{0.4}RhIn_5$.

Correa V.F., Tung L., Hollen S.M., Pagliuso P.G., Moreno N.O., Lashley J.C., Sarrao J.L., and Lacerda A.H.

We report thermal-expansion and magnetostriction results on Ce0.6La0.4RhIn5 single crystals. This particular La concentration (x_c~0.4) corresponds to the critical one at which the long-range magnetic order vanishes (T_N=0). However, as also observed in specific heat and magnetic susceptibility measurements, a large *"hump"* is seen in thermal-expansion at T_{SR} ~ 4.5 K. This anomaly, claimed to be related to short-range correlations, is observed only along the c-axis, confirming that anisotropy plays an important role in these 115 compounds. No particular feature is associated with the magnetic correlations in the magnetostriction measurements. The magnetic field dependence of the volume is quadratic in field as expected for a paramagnetic system, above and below T_{SR}. Finally, the magnetic field dependence of the crystal electric field contribution to the thermal-expansion seems to reinforce the idea that the La doping leads to a |±5/2>-rich ground state doublet.

Physical Review B, accepted on March 2004.

A 016- 04 Anomalous *f*-electron Hall Effect in the Heavy-Fermion System $CeTIn_5$ (T = Co, Ir, or Rh).

Hundley M.F., Malinowski A., Pagliuso P.G., Sarrao J.L., and Thompson J.D.

The in-plane Hall coefficient $R_H(T)$ of $CeRhIn_5$, $CeIrIn_5$, and $CeCoIn_5$ and their respective non-magnetic lanthanum analogs are reported in fields to 90 kOe and at temperatures from 2 K to 325 K. $R_H(T)$ is negative, field-independent, and dominated by skew-scattering above ~ 50 K in the Ce compounds. $R_H(H ? 0)$ becomes increasingly negative below 50 K and varies with temperature in a manner that is inconsistent with skew scattering. Field-dependent measurements show that the low-T anomaly is strongly suppressed when the applied field is increased to 90 kOe. Measurements on $LaRhIn_5$, $LaIrIn_5$, and $LaCoIn_5$ indicate that the same anomalous temperature dependence is present in the Hall coefficient of these non-magnetic analogs, albeit with a reduced amplitude and no field dependence. Hall angle ($\dot{e}_H$) measurements find that the ratio $\tilde{n}_{xx}/\tilde{n}_{xy} = \cot(\dot{e}_H)$ varies as T^2 below 20 K for all three Ce-115 compounds. The Hall angle of the La-115 compounds follow this T-dependence as well. These data suggest that the electronic-structure contribution dominates the Hall effect in the 115 compounds, with *f*-electron and Kondo interactions acting to magnify the influence of the underlying complex band structure. This is in stark contrast to the situation in most 4*f* and 5*f* heavy-fermion compounds where the normal carrier contribution to the Hall effect provides only a small, T-independent background to R_H.

Physical Review B, accepted on May 2004.

A 017 - 04 "Origin of the A_{1g} Electronic Raman Scattering Peaks in the Superconducting State of $YBa_2Cu_3O_{7-}d$.

Martinho H., Martin A.A., Rettori C. and Lin C.T.

The electronic Raman scattering was investigated in optimally oxygen-doped $YBa_2Cu_3O_{7-}d$ single crystals as well in crystals doped with nonmagnetic, Zn^{2+} and magnetic Ni^{2+} impurities. We found that the intensity of the A_{1g} peak is impurity independent and its energy to T_c ratio is nearly constant ($2D/k_BT_c$~5). Moreover, the signal at the B_{1g} channel is completely smeared out when nonmagnetic Zn^{2+} impurities are present. These results are discussed in terms of the current models of Devereaux et al., Venturini et al., and Zeyher and Greco.

Physical Review B 69 [1805XX(R)] , accepted on May 2004.

A 018-04 Rare earth doped silicon nanocrystals derived from an erbium amidinateprecursor.

Jumin Ji1, Robert A Senter1, Leandro R Tessler2, Dwayne Back3,Charles H Winter3 and Jeffery L Coffer1

We describe the use of Er(tBuNC(CH3)NtBu)3 as a dopant source in the preparation of silicon nanocrystals, particularly as regards their observed structure, composition, and photophysical properties. These nanocrystals were prepared by the co-pyrolysis of Er(tBuNC(CH3)NtBu)3 and disilane in a dilute helium stream at 1000 ?C. Characterization methods include high resolution electron microscopy, selected area electron diffraction, energy dispersive x-ray measurements, extended x-ray absorption spectroscopy, and photoluminescence spectroscopy. In conditions identical to those used previously for â-diketonate precursors, nanocrystals doped using this amidinate source are larger in size, of a narrower size distribution, and contain more erbium in the nanocrystal on average. Steady state photoluminescence measurements as a function of excitation wavelength confirm that the characteristic 1540 nm emission detected in these nanocrystals emit by a silicon exciton-mediated pathway. These results are a clear example of precursor dopant chemistry exerting a significant effect on resultant nanoparticle properties.

Nanotechnology 15 (2004) 643-647 PII: S0957-4484(04)74590-0, accepted on May 2004.

LIVRO NO PRELO

L 001- 04 Ensemble formalisms for nonequilibrium systems and an associated irreversible statistical thermodynamics

A. R. Vasconcellos, J. Galvão Ramos, and R. Luzzi

It is reviewed what can be considered as the present research trends in what regards to the construction of an ensemble formalism- Gibbs´style- for the case of far-from-equilibrium systems. The main questions involved are presented accompanied with brief discussions. The construction of a nonequilibrium statistical operator is described and its applications commented, and, particularly, it is presented the derivation of an Irreversible Thermodynamics based on the statistical foundations that the nonequilibrium ensemble

formalism provides

"Trends in Statistical Physics`` (Renew Series Research Trends) accepted on May 2004.

Trabalhos Publicados

P 053- 04 "Breaking of gold nanowires".

da Silva, E. Z., da Silva, A. J. R., and Fazzio, A

We have investigated the formation evolution and breaking of a gold nanowire using molecular dynamics simulation. Results reproduce many features observed experimentally. Suspended gold nanowires have recently been produced in an ultra-high vacuum and were imaged by electron microscopy. Here we simulate gold nanowires under stress. In particular, we discuss the mechanisms of formation, evolution and breaking of these atomically thin Au nanowires. (C) 2004 Elsevier B.V. All rights reserved

Computational Materials Science **30[1-2], 73-76. 2004.**

P 054- 04 "Carbon nanotube probe resolution: a quantitative analysis using Fourier Transform".

Gutierrez, H. R., Nakabayashi, D., Silva, P. C., Bortoleto, J. R. R., Rodrigues, V., Clerici, J. H., Cotta, M. A., and Ugarte, D.

A method to quantify the resolution of atomic force microscopy (AFM) probes using Fourier analysis of the AFM images is, proposed. The maximum detectable spatial frequency obtained from the power spectrum was used to estimate the lateral resolution. Carbon nanotube tips were successfully used to study very dense arrays of semiconductor nanostructures. In particular, accurate measurements of shallow facet angles were obtained, which are in perfect agreement with results obtained by two complementary techniques - High Resolution Transmission Electron Microscopy and Reflection High-Energy Electron Diffraction. (C) 2004 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

Physica Status Solidi A-Applied Research **201[5], 888-893. 2004.**

P 055- 04 "Considerations on undistorted-progressive X-waves and Davydov solitons, Frohlich-Bose-Einstein condensation, and Cherenkov-like effect in biosystems".

Mesquita, M. V., Vasconcellos, A. R., and Luzzi, R

Research in ultrasonography has evidenced the propagation of a peculiar kind of excitation in fluids. Such excitation, dubbed a X-wave, has characteristics resembling that of a solitary-wave type. We reconsider the problem in a medium consisting of a biological material of the like of a-helix proteins. It can be shown that in this case is expected an excitation of the Davydov's solitary wave type, however strongly damped in normal conditions. The case of acetanilide, an organic polymer which resembles biopolymers, is considered, and the infrared spectrum analyzed. Davydov's soliton is evidenced as a coherent state of polar vibrations. The case of acoustic (sound) vibrations is also considered, where, also, a damped Davydov-like solitary wave may be excited. However, it is shown that when traveling in conditions sufficiently away from equilibrium, more precisely, when the soliton is embeded in the resulting Frohlich-Bose-Einstein condensate, the lifetime of the solitary wave is largely enhanced. Moreover, a soliton moving in bulk with a velocity larger than that of the group velocity of the normal vibrational waves would produce a Cherenkov-like emission of phonons giving rise to the observed X-wave-like pattern. This paper is a modified and extended version of an earlier publication on the subject.

Brazilian Journal of Physics **34[2A], 489-503. 2004.**

P 056- 04 "Correlations between total cross sections and slopes".

Martini, A. F., Menon, M. J., and Montanha, J.

We investigate correlations between the total cross section and the slope of the elastic differential cross section for proton-proton and antiproton-proton scattering at the highest energies. Based on the empirical behavior of these quantities as function of the energy, we select two different analytical parametrizations connecting them, and obtain the correlations through fits to the experimental data available. We present and discuss practical uses of extrapolations and interpolations of the results. In the former case we refer to the estimation of the proton-proton total cross sections from the proton-air cross sections (obtained from cosmic-ray experiments), and in the later case, we critically discuss the recent measurement of the slope parameter at the BNL RHIC at 200 GeV by the pp2pp Collaboration

Brazilian Journal of Physics **34[1A], 263-267. 2004.**

P 057- 04 "Domain-wall scattering in an interacting one-dimensional electron gas".

Pereira, R. G. and Miranda, E.

We study the transport in a Luttinger liquid coupled to a magnetic chain containing a Bloch domain wall. We compute the leading correction to the adiabatic limit of a long domain wall, which causes no scattering. We show that the problem is reminiscent of an impurity in a Luttinger liquid, but with a different dependence on the interaction parameters due to spin-flip scattering. For repulsive interactions, we find that the domain-wall resistance diverges with decreasing temperature. This may be relevant for the design of one-dimensional systems with large magnetoresistance at low temperatures

Physical Review B **69[14]. 2004.**

P 058- 04 "Dynamics of topological defects in a spiral: A scenario for the spin-glass phase of cuprates".

Juricic, V., Benfatto, L., Caldeira, A. O., and Smith, C. M.

We propose that the dissipative dynamics of topological defects in a spiral state is responsible for the transport properties in the spin-glass phase of cuprates. Using the collective-coordinate method, we show that topological defects are coupled to a bath of magnetic excitations. By integrating out the bath degrees of freedom, we find that the dynamical properties of the topological defects are dissipative. The calculated damping matrix is related to the in-plane resistivity, which exhibits an anisotropy and linear temperature dependence in agreement with experimental data

Physical Review Letters **92[13]. 2004.**

P 059- 04 "Electromagnetic response of layered superconductors with broken lattice inversion symmetry".

Uchoa, B., Neto, A. H. C., and Cabrera, G. G.

We investigate the macroscopic effects of charge-density waves (CDW) and superconductivity in layered superconducting systems with broken lattice inversion symmetry (allowing for piezoelectricity) such as two-dimensional transition metal dichalcogenides. We work with the low-temperature time-dependent Ginzburg-Landau theory and study the coupling of lattice distortions and low-energy CDW collective modes to the superconducting order parameter in the presence of electromagnetic fields. We show that superconductivity and piezoelectricity can coexist in these singular metals. Furthermore, our study indicates the nature of the quantum phase transition between a commensurate CDW phase and the stripe phase that has been observed as a function of applied pressure

Physical Review B **69[14]. 2004.**

P 060- 04 "Electron-impact excitation of H-2: minimal orbital basis for single configuration interaction".

da Costa, R. F., da Paixao, F. J., and Lima, M. A. P.

We report theoretical differential excitation cross sections for scattering of electrons by H-2 molecules using the Schwinger multichannel approach (SMC). This study differs from previous applications of the SMC method in the description of the excited states (which are now obtained through the single configuration 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 significant improvement to experimental data in comparison with earlier two-state close coupling calculations.

Journal of Physics B-Atomic Molecular and Optical Physics **37[6], L129-L135. 2004.**

P 061- 04 "Electron collisions with isomers of C4H8 and C4H10".

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

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 C-2h 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 CnHm molecules (with combinations of n = 1, 2, 3, 4 and m = 2, 4, 6, 8, 10).

Journal of Physics B-Atomic Molecular and Optical Physics **37[5], 997-1012. 2004.**

P 062- 04 "Electronic excitation of N-2 by positron impact".

Chaudhuri, P., Varella, M. T. D., de Carvalho, C. R. C., and Lima, M. A. P.

We present cross sections of electronic excitation of nitrogen molecule (N-2) by positron impact using the Schwinger multichannel method. Our calculated cross sections are compared with the recent and the only available experimental data of Sullivan [Phys. Rev. Lett. 87, 073201 (2001)] . Present theoretical results for excitation to the a (1)Pi(g) states do not reproduce the near-threshold structure observed in the experimental data.

Physical Review A **69[4]. 2004.**

P 063- 04 "Electronic structure and origin of ferromagnetism in Ga1-xMnxAs semiconductors".

da Silva, A. J. R., Fazzio, A., dos Santos, R. R., and Oliveira, L. E.

We perform a detailed theoretical study, within the density-functional theory, of the electronic structure and magnetic properties of Ga1-xMnxAs diluted semiconductors. Ab initio total energy results provide evidence that the appearance of a ferromagnetic state in these materials is due to an exchange coupling between the localized up arrow S =5/2 Mn spins mediated by quasi-localized down arrow holes, with strong p-like character, surrounding the fully polarized Mn d(5)-electrons. From total energy differences, we find the effective Mn-Mn coupling always ferromagnetic, with the Mn-Mn interaction intermediated by an anti ferromagnetic coupling of each Mn spin to the holes.

Physica B-Condensed Matter **340, 874-877. 2003.**

P 064- 04 "Electronic, structural, and magnetic properties of cobalt aggregates embedded in polypyrrole".

Watanabe, N., Morais, J., Accione, S. B. B., Morrone, A., Schmidt, J. E., and Alves, M. C. M.

In this paper, we report on the synthesis and characterization of cobalt aggregates electrochemically incorporated on composite polypyrrole films. XAS (X-ray absorption spectroscopy) was used to probe the atomic local order in these composites and to furnish new insights into the metal/polymer interaction. A complete understanding of the incorporation process and its evolution was achieved by in situ XAS measurements at different stages of the electrochemical process. These results indicate that the reaction starts with the Co2+ entrapped in the polymeric matrix as a complex [-[(C4H2N)(3)CH3(CH2)(11)OSO3-](6)CO2+]. The reduction of this complex leads to the synthesis of Co aggregates in the film. Measurements at the O and N K edges evidence that the main interaction between Co aggregates and the polymer is verified via Co-N bonds, the N originating from the polypyrrole (PPy) amine group. The pH effect on the metal/polymer interaction is discussed. Scanning electron microscopy (SEM) measurements show the formation of dendritic-like cobalt aggregates on the film surface. The magnetic response obtained by in situ alternating gradient field magnetometry (AGFM) allows prediction of the possibility of obtaining a magnetic polymer with superparamagnetic particles with sizes below 10 nm. Our results are the first steps toward the development of an advanced material with exciting potential for future recording media application.

Journal of Physical Chemistry B **108[13], 4013-4017. 2004.**

P 065- 04 "Entanglement versus chaos in disordered spin chains".

Santos, L. F., Rigolin, G., and Escobar, C. O.

We use a Heisenberg spin-1/2 chain to investigate how chaos and localization may affect the entanglement of pairs of qubits. To measure how much entangled a pair is, we compute its concurrence, which is then analyzed in the delocalized (localized) and in the chaotic (nonchaotic) regimes. Our results indicate that chaos reduces entanglement and that entanglement decreases in the region of strong localization. In the transition region from a chaotic to a nonchaotic regime localization increases entanglement. We also show that entanglement is larger for strongly interacting qubits (nearest neighbors) than for weakly interacting qubits (next and next-next neighbors)

Physical Review A 69[4]. 2004.

P 066- 04 "EXAFS investigation of local structure of Er3+ and Yb3+ in low-silica calcium aluminate glasses".
Sampaio, J. A. and Gama, S

Erbium and ytterbium environments in low-silica calcium aluminate glasses, with nominal composition 58 CaO, 27.1-x Al2O3, 6.9 MgO, 8 SiO2, x Er2O3, or Yb2O3, 0.2less than or equal toxless than or equal to1.5 (mol %), were investigated using x-ray-absorption fine-structure spectroscopy (EXAFS) on the Er and Yb L-III edge. The average Er-O bond separation was found to vary only slightly between 2.24 and 2.21 Angstrom and the Yb-O bond between 2.20 and 2.18 Angstrom. The first-shell coordination number decreased as the rare-earth oxide replaced Al2O3. For Er2O3-doped samples this decrease was about 28%, from 6.5 to 4.7 atoms, whereas for Yb2O3-doped ones it was about 14%, from 6.4 to 5.5 atoms. The decrease in the coordination number is attributed to the difficulty of rare-earth atoms to coordinate a larger number of the nonbridging oxygens that appear as the CaO/Al2O3 ratio decreases. The Debye-Waller factor 2sigma(2) varied from 0.026 to 0.012 Angstrom(2)
***Physical Review B* 69[10]. 2004.**

P 067- 04 "Exciton trapping in interface defects/quantum dots in narrow quantum wells: magnetic-field effects".
Barticevic, Z., Pacheco, M., Duque, C. A., and Oliveira, L. E

The effects of applied magnetic fields on excitons trapped in quantum dots/interface defects in narrow GaAs/ Ga1-xAlxAs quantum wells are studied within the effective-mass approximation. The magnetic fields are applied in the growth direction of the quantum wells, and exciton trapping is modeled through a quantum dot formed by monolayer fluctuations in the z-direction, together with lateral confinement via a truncated or infinite parabolic potential in the exciton in-plane coordinate. Theoretical results are found in overall agreement with available experimental measurements. (C) 2003 Elsevier B.V. All rights reserved
***Physica B-Condensed Matter* 340, 1090-1093. 2003.**

P 068- 04 "Extensions of the extrema bounds for the pomeron intercept to meson-proton, gamma-proton and gamma-gamma scattering".
Luna, E. G. S., Menon, M. J., and Montanha, J.
Making use of the extrema bounds for the soft pomeron intercept, recently determined by fits to pp and pp data (from both accelerator and cosmic-ray experiments), we investigate the total cross sections for pion-proton, kaon-proton, gamma-proton and gamma-gamma scattering. We show that by means of global fits, the extrema bounds are in agreement with the bulk of experimental data presently available, and that extrapolations to higher energies indicate different behaviors for the rise of the total cross sections. We also discuss factorization and quark counting, showing that both bounds are in agreement with these properties
***Brazilian Journal of Physics* 34[1A], 268-271. 2004.**

P 069- 04 "FIR laser lines from CH3OD: A review".
De Michele, A., Carelli, G., Moretti, A., Pereira, D., Costa, L. F., Cruz, F. C., and Moraes, J. C. S.
The methanol isotopic species CH3OD has also proved to be an efficient and powerful medium to generate radiation in the far infrared (FIR) region. After the critical review of 1994, six papers have been published dealing with new FIR laser lines from this molecule. As a consequence of the use of wide tunability waveguide CO2 lasers as well as a new pulsed CO2 laser operating at hot and sequential bands, as of optical pumping sources, the total number of the FIR laser lines increased from 122 in 1994 to 227 today. In this communication we present an updated and complete catalogue of FIR laser lines generated from CH3OD. Information on wavelength, offset, relative polarization, intensity, and optimum operation pressure is generally available
***International Journal of Infrared and Millimeter Waves* 25[5], 725-734. 2004.**

P 070- 04 "Fixation of beneficial mutations in the presence of epistatic interactions".
Campos, P. R. A.
We investigate the effect of deleterious mutations on the process of fixation of new advantageous mutants in an asexual population. In particular we wish to study the dependence of the process on the strength of the deleterious mutations. We suppose the existence of epistatic interaction between the genes. We study the model by means of branching process theory and also by numerical simulations. Our results show the occurrence of two distinct regimes of behavior for the probability of fixation of these variants. The occurrence of either regime depends on the ratio between the selective advantage of the beneficial mutation s(b) and on the selective parameter for deleterious mutations s(d). In the former, which takes place for s(b)/s(d) less than or similar to 1, the probability of fixation increases with the epistasis parameter alpha, whereas for s(b)/s(d) much greater than 1 the probability of fixation is a complex function of alpha and the mutation rate U. Surprisingly, we find that for the multiplicative landscape (alpha = 1) the probability of fixation P-fix is given by P-fix = pi(s(b))e(-U/sd) where pi(s(b)) is the probability of fixation for the two-allele model in the absence of mutations as calculated by Haldane (1927, Proc. Camb. Phil. Soc., 26, 220-230) and Kimura (1962, Genetics, 47, 713-719). (C) 2003 Society for Mathematical Biology. Published by Elsevier Ltd.
***Bulletin of Mathematical Biology* 66[3], 473-486. 2004.**

P 071- 04 "Gigahertz nanomechanical oscillators based on carbon nanotubes".
Legoas, S. B., Coluci, V. R., Braga, S. F., Coura, P. Z., Dantas, S., and Galvao, D. S

We report molecular dynamics studies of carbon nanotubes as mechanical gigahertz oscillators. Our results show that different oscillatory regimes exist but that sustained oscillations are possible only when the radii difference values of the inner and outer tubes are similar to3.4 Angstrom. Frequencies as large as 87 GHz were obtained. Calculated force and frequency values are in good agreement with estimated data from recent experimental investigations
***Nanotechnology* 15[4], S184-S189. 2004.**

P 072- 04 "Hole mobility in zincblende c-GaN".
Rodrigues, C. G., Fernandez, J. R. L., Leite, J. R., Chitta, V. A., Freire, V. N., Vasconcellos, A. R., and Luzzi, R.

We consider the nonequilibrium thermodynamic state of carriers in III-nitrides, and calculate the mobility of holes in cubic GaN layers under electric fields of low intensity. The contribution of different scattering mechanisms to the mobility is analyzed, and the relevance of each one is characterized. Satisfactory agreement with recently published experimental data is obtained.
***Journal of Applied Physics* 95[9], 4914-4917. 2004.**

P 073- 04 "Infrared and Raman studies on films of organosiloxane networks produced by PECVD".
Trasferetti, B. C., Davanzo, C. U., and de Moraes, M. A. B.

The effect of the incorporation of oxygen and nitrogen on the structure of films obtained by PECVD of hexamethyldisiloxane (HMDSO)-He-N-2 and HMDSO-He-O-2 mixtures is investigated using infrared and Raman spectroscopies. From transmittance spectra of films deposited onto single-crystal KBr disks, the transverse optical (TO) and longitudinal optical (LO) functions in the mid-infrared region were calculated. To correlate structural aspects with the observed LO-TO splittings, an identification analysis of functional group based on the infrared and Raman literature was made. It was concluded that the structure of the films deposited from HMDSO-He-O-2 discharges was strongly dependent on the proportion of oxygen in the gas feed. In the absence of oxygen, i.e., for a discharge of a HMDSO-He mixture, the resulting film consisted of a network of interconnected siloxane and carbosilane units. Addition of O-2 precluded the formation of methylene bridges and induced the formation of a material enriched with Si-O-Si groups. Films formed from the HMDSO-He-N-2 plasmas, on the other hand, consisted mainly of interconnected siloxane and carbosilane units in addition to a small quantity of silazane units. On the basis of these results, we propose an interpretation for the variation of the LO-TO splitting amplitude for the asymmetrical stretching mode (AS1) of Si-O in Si-O-Si groups as a function of the oxygen or nitrogen incorporation into the films.

***Macromolecules* 37[2], 459-466. 2004.**

P 074- 04 "Interaction between superconducting and ferromagnetic order parameters in graphite-sulfur composites".
Moehlecke, S., Kopelevich, Y., and Maple, M. B

The superconductivity of graphite-sulfur composites is highly anisotropic and associated with the graphite planes. The superconducting state coexists with the ferromagnetism of pure graphite, and a continuous crossover from superconducting to ferromagneticlike behavior could be achieved by increasing the magnetic field or the temperature. The angular dependence of the magnetic moment m(alpha) provides evidence for an interaction between the ferromagnetic and the superconducting order parameters.
Physical Review B **69[13]. 2004.**

P 075- 04 "Interaction of argon clusters with intense VUV-laser radiation: The role of electronic structure in the energy-deposition process".
Laarmann, T., de Castro, A. R. B., Gurtler, P., Laasch, W., Schulz, J., Wabnitz, H., and Moller, T.

The response of Ar clusters to intense vacuum-ultraviolet pulses is investigated with photoion spectroscopy By varying the laser wavelength, the initial excitation was either tuned to absorption bands of surface or bulk atoms of clusters. Multiple ionization is observed, which leads to Coulomb explosion. The efficiency of resonant 2-photon ionization for initial bulk and surface excitation is compared with that of the norresonant process at different laser intensities. The specific electronic structure of clusters plays almost no role in the explosion dynamics at a peak intensity larger than 1.8 X 10(12) W/cm(2). The inner ionization of atoms for resonant and nonresonant excitation is then saturated and the energy deposition is mainly controlled by the plasma heating rate. Molecular dynamics simulations indicate that standard collisional heating cannot fully account for the strong energy absorption.
Physical Review Letters **92[14]. 2004.**

P 076- 04 "Invasion and extinction in the mean field approximation for a spatial host-pathogen model".
de Aguiar, M. A. M., Rauch, E. M., and Bar-Yam, Y.

We derive the mean field equations of a simple spatial host-pathogen, or predator-prey, model that has been shown to display interesting evolutionary properties. We compare these equations, and the equations including pair-correlations, with the low-density approximations derived by other authors. We study the process of invasion by a mutant pathogen, both in the mean field and in the pair approximation, and discuss our results with respect to the spatial model. Both the mean field and pair correlation approximations do not capture the key spatial behaviors-the moderation of exploitation due to local extinctions, preventing the pathogen from causing its own extinction. However, the results provide important hints about the mechanism by which the local extinctions occur.
Journal of Statistical Physics **114[5-6], 1417-1451. 2004.**

P 077- 04 "Local effects in strained marnganite thin films".

Souza-Neto, N. M., Ramos, A. Y., Tolentino, H. C. N., Favre-Nicolin, E., and Ranno, L.

We report on polarized X-ray absorption spectroscopy (P-XAS) study of La0.7Sr0.3MnO3 (LSMO) films, epitaxially grown by laser ablation on tensile (SrTiO3) and compressive (LaAlO3) substrates. In-plane and out-of-plane bond information was obtained by setting the angle between electric field vector and film surface close to 0 and 90degrees, respectively. Measurements show significant modifications in the average MnO6 octahedron around manganese atoms in the film plane for tensile and compressive substrates. The modifications of the XANES spectra were correlated to a modification in the average Mn-O distance and a distortion of the MnO6 octahedra. Ab initio calculations using the full multiple scattering approach confirm the structural model of distorted octahedron.
Journal of Alloys and Compounds **369[1-2], 205-208. 2004.**

P 078- 04 "Magnetic structure and fluctuations of Gd2IrIn8: A resonant x-ray diffraction study".
Granado, E., Pagliuso, P. G., Giles, C., Lora-Serrano, R., Yokaichiya, F., and Sarrao, J. L.

Resonant x-ray diffraction measurements on Gd2IrIn8 reveal an antiferromagnetic structure below T-N=40.8 K with wave vector zeta=(1/2,0,0) and the Gd moments lying in the tetragonal ab plane, indicating partly frustrated exchange interactions. Strong (over three orders of magnitude) dipolar resonant enhancements of the magnetic reflections were observed at both Gd L-II and L-III edges, indicating a relatively high magnetic polarization of the Gd 5d levels. Three-dimensional magnetic fluctuations are evidenced below T-N, while measurements taken slightly above T-N are consistent with two coexisting length scales for the magnetic correlations. Implications of these results for the physics of CenMmIn3n+2m (M=Co, Rh, or Ir) heavy-fermion superconductors are discussed.
Physical Review B **69[14]. 2004.**

P 079- 04 "Magneto-impedance measurements in bulk samples of La0.7Ca0.3MnO3 and La0.6Y0.1Ca0.3MnO3".
Castro, G. M. B., Rodrigues, A. R., Machado, F. L. A., de Araujo, A. E. P., Jardim, R. F., and Nigam, A. K

In this work, magneto-resistance and magneto-impedance (MI) data for bulk samples of pure and Y-doped La0.7Ca0.3MnO3 manganites are reported. Temperature dependent measurements were carried out sweeping the applied magnetic field H in the -6 T < H < 6 T range. The measurements were done with do and ac electrical currents, varying the frequencies f up to 5 MHz, using a four-probe technique. The pure La0.7Ca0.3MnO3 sample presented a metal-insulator-transition near the ferromagnetic transition (T-C = 245 K). For these samples, magneto-resistance of the order 60% for H = 6 T was observed close to T-C. The substitution of ions of La by Y (La0.6Y0.1Ca0.3MnO3) reduced T-C to 170 K but, on the other hand, increased the magneto-resistance to over 90% near T-C. In the measurements with ac currents, the data for both samples presented a large magneto-impedance effect. The MI is more pronounced at high fields and for the Y-doped samples. Moreover, the Y-doped samples showed a strong hysteretic behavior that was not observed in the pure samples.
Journal of Alloys and Compounds **369[1-2], 108-111. 2004.**

P 080- 04 "Manufacturing the Schmidt corrector lens for the Pierre Auger Observatory".
de Oliveira, M. A. L., de Souza, V., Reis, H. C., and Sato, R.

The Pierre Auger Observatory is designed to provide measurements of Extensive Air Showers initiated in the upper atmosphere by cosmic rays with energies greater than 10(18) eV. One of the employed techniques is air fluorescence detectors with UV filters and a corrector lens. We describe in this article the production process of the corrector lens in Brazil, starting from the design of the machines up to the final tests in the prototype telescope. We have used diamond grinding tools to shape a ring of corrector lens with inner radius of 85 cm and outer radius of I 10 cm, divided in 24 segments and with aspherical shape. After the production of a first complete set of segments, we measured a segment shape scanning with a laser. The lens was then installed at the telescope and we measured its overall influence on the spot size, taking pictures of the Vega star.
Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment **522[3], 360-370. 2004.**

P 081- 04 "Mechanical properties of nanosprings"..

da Fonseca, A. F. and Galvao, D. S.

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

Physical Review Letters **92[17]. 2004**

P 082- 04 "Molybdenum oxide thin films obtained by the hot-filament metal oxide deposition technique".

de Moraes, M. A. B., Trasferetti, B. C., Rouxinol, F. P., Landers, R., Durrant, S. F., Scarminio, J., and Urbano, A.

Molybdenum oxide thin films find diverse applications as catalysts, gas sensors, and electrochromic devices. Such films are produced mainly by reactive sputtering and thermal evaporation but other techniques such as chemical vapor deposition and electrochemical deposition have been used. In the present work, the feasibility of an alternative method for the production of molybdenum oxide films using a molybdenum filament heated in a rarefied oxygen atmosphere is demonstrated. The filament heating current, IF, and the oxygen flow rate, F-O\2, are the key deposition parameters and their effect on the deposition rate, R, was investigated. For I-F = 12.5 A, an increase in the R-value from 7.5 to 31 nm/min was observed as FO2 was increased from 6.0 to 21 sccm. To characterize the chemical bonds, infrared spectroscopy, using both unpolarized and p-polarized infrared beams, and X-ray photoelectron spectroscopy (YPS) were employed. Line shape analysis of the Mo(3d) XPS peak revealed that the Mo atoms were in mixed valence states, Mo6+ and Mo5+, with a high predominance of the former over the latter, thus indicating an oxygen-deficient MoO3 film. From Rutherford backscattering spectroscopic analysis of the films, an average O/Mo atomic ratio of 2.9 was calculated, consistent with the XPS results. A combination of the XPS and RBS results and the data of other investigators on the oxidation of molybdenum suggests that the film is formed from MoO2 and MoO3 species desorbed from the Mo filament. The optical gap, E-g, was determined from transmission UV-visible spectra of the films. An average E-g value of 3.03 eV was found. The electrochromic properties of the films were investigated for Li+ intercalation using an electrochemical cell. A coloration efficiency of 19.5 cm(2)/C at a wavelength of 700 nm was observed.
Chemistry of Materials **16[3], 513-520. 2004.**

P 083- 04 "New families of carbon nanotubes based on graphyne motifs".

Coluci, V. R., Braga, S. F., Legoas, S. B., Galvao, D. S., and Baughman, R. H.

Electronic properties of proposed new families of carbon single walled nanotubes are investigated. These nanotubes, called graphynes, result from the elongation of covalent interconnections of graphite-based nanotubes by the introduction of yne groups. Analogous to ordinary nanotubes, armchair, zigzag and chiral graphyne nanotubes are possible. Tight-binding and ab initio density functional methods were used to predict the electronic properties of these unusual nanotubes. Of the three graphyne nanotube families analysed here, two provide metallic behaviour for armchair tubes and either metallic or semiconducting behaviour for zigzag nanotubes. For the other graphyne nanotube family investigated a diameter and chirality independent bandgap is predicted and a bandgap modulation study by structural distortions has been carried out for small longitudinal tube deformations. Interestingly, while the bandgap is insensitive to structure, the stress-induced bandgap changes can strongly depend both on the nanotube type and whether the strain is tensile or compressive.
Nanotechnology **15[4], S142-S149. 2004.**

P 084- 04 "Non-linear magetoinductance in amorphous wires".
Clime, L., Rudkowska, G., Duque, J. G. S., de Araujo, A. E. P., Knobel, M., Ciureanu, P., and Yelon, A.

The second harmonic of the magneto inductance (MI) signal of a melt-extracted amorphous magnetic wire varies significantly with the strength of the DC axial field applied to the wire. Its amplitude at frequencies between 200 kHz and I MHz was measured with a spectrum analyzer. We found that it has a four-peak structure, and that the peak amplitude increases with the frequency of the driving current. When a tensile stress is applied to the wire, the central peaks diminish, while the outer peaks are more widely spaced on the field axis. A simple analytical model of the MI signal shows that a large second harmonic of this signal and a large asymmetry in the circumferential hysteresis loop of the wire occur together and are manifestations of the same material property.

Physica B-Condensed Matter **343[1-4], 410-414. 2004.**

P 085- 04 "Phase diagram and critical behavior of the spin-1 Baxter-Wu model with a crystal field".

Costa, M. L. M., Xavier, J. C., and Plascak, J. A.

The phase diagram and critical behavior of the spin-1 Baxter-Wu model with a crystal field in two dimensions is explored by renormalization group, conventional finite-size scaling, and conformal invariance techniques. We found that the phase diagram of this model is qualitatively the same as that of the dilute 4-states Potts model, presenting a multicritical point for a finite value of the crystal field, in disagreement with previous work based on finite-size calculations. However, our results indicate that the critical exponents vary continuously along the second-order transition line, differently from the expected behavior of the dilute 4-states Potts model.

Physical Review B **69[10]. 2004**

P 086- 04 "Properties and performance of the prototype instrument for the Pierre Auger Observatory".

Abraham, J., et al...

Construction of the first stage of the Pierre Auger Observatory has begun. The aim of the Observatory is to collect unprecedented information about cosmic rays above 10(18) eV. The first phase of the project, the construction and operation of a prototype system, known as the engineering array, has now been completed. It has allowed all of the sub-systems that will be used in the full instrument to be tested under field conditions. In this paper, the properties and performance of these sub-systems are described and their success illustrated with descriptions of some of the events recorded thus far.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment **523[1-2], 50-95. 2004.**

P 087- 04 "Specific heat at high temperature and magnetic measurements in Nd0.5Sr0.5MnO3 and R0.5Ca0.5MnO3 (R = Nd, Sm, Dy and Ho) samples".

Lopez, J. and de Lima, O. F.

We have made a magnetic and specific heat characterization of five manganese samples. Ferromagnetic, antiferromagnetic and charge ordering transitions in our samples agree with previous reports. Each specific heat curve was successfully fitted at high temperatures by an Einstein model with three optical phonon modes. Close to the charge ordering and ferromagnetic transition temperatures the specific heat curves showed peaks superposed to the characteristic response of the lattice oscillations.
Journal of Alloys and Compounds **369[1-2], 227-230. 2004.**

P 088- 04 "Structure and dynamics of carbon nanoscrolls".
Braga, S. F., Coluci, V. R., Legoas, S. B., Giro, R., Galva, D. S., and Baughman, R. H.

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 find that charge injection causes unwinding of the CNSs, which might be important for the application of CNSs as nanomechanical actuators.
***Nano Letters* 4[5], 881-884. 2004.**

P 089- 04 "Substrate-induced strain effects on Pr0.6Ca0.4MnO3 films".

Nelson, C. S., Hill, J. P., Gibbs, D., Rajeswari, M., Biswas, A., Shinde, S., Greene, R. L., Venkatesan, T., Millis, A. J., Yokaichiya, F., Giles, C., Casa, D., Venkataraman, C. T., and Gog, T

We report the characterization of the crystal structure, low-temperature charge and orbital ordering, transport and magnetization of Pr0.6Ca0.4MnO3 films grown on LaAlO3, NdGaO3 and SrTiO3 substrates, which provide compressive (LaAlO3) and tensile (NdGaO3 and SrTiO3) strain. The films are observed to exhibit different crystallographic symmetries from the bulk material and the low-temperature ordering is found to be more robust under compressive-as opposed to tensile-strain. In fact, bulk-like charge and orbital ordering is not observed in the film grown on NdGaO3, which is the substrate that provides the least amount of measured, but tensile, strain. This result suggests the importance of the role played by the Mn-O-Mn bond angles in the formation of charge and orbital ordering at low temperatures. Finally, in the film grown on LaAlO3, a connection between the lattice distortion associated with orbital ordering and the magnetization is reported

***Journal of Physics-Condensed Matter* 16[1], 13-27. 2004.**

P 090- 04 "Systems biology: An information-theoretic-based thermo-statistical approach".
Mesquita, M. V., Vasconcellos, A. R., Luzzi, R., and Mascarenhas, S.

Systems Biology (system-level understanding in biological science), from the physical-chemical point of view, is involved with irreversible thermodynamics and nonlinear kinetic theory of open systems which are founded on nonequilibrium statistical mechanics. We describe a modern thermo-statistical approach for dealing with complex systems, in particular biological systems. We consider the case of a very peculiar complex behavior in open boson systems sufficiently away, from equilibrium, which appear to have large relevance in the functioning of biological systems. This is, on the one hand, the so-called Frohlich-Bose-Einstein-like condensation leading in steady-state conditions to the emergence of a particular case of quantum-large-scale coherent ordering, of the type of a selforganizing-synergetic dissipative structure. Moreover, additional complexity emerges in the form of propagation, in this condensate, of signals (information) consisting of nearly undamped and undistorted, long-distance propagating, solitary waves (the pseudoparticle soliton). It can be accompanied by a so-called Frohlich-Cherenkov cone of emission of polar vibrations, and it is also possible the formation of metastable states of the form of the so-called bioelectrets. These are phenomena apparently working in biological processes, which are presently gaining relevant status on the basis of eventually providing a large-scale quantum-coherent behavior in cytoskeletons of neurons and the conscious (non-computational) activity in the brain. Emphasis is centered on the quantum-mechanical-statistical irreversible thermodynamics of these open systems, and the informational characteristics of the phenomena. Ways for their experimental evidencing are pointed out and discussed.

***Brazilian Journal of Physics* 34[2A], 459-488. 2004.**

P 091- 04 "Testing the magnetism of polymerized fullerene".

Boukhvalov, D. W., Karimov, P. F., Kurmaev, E. Z., Hamilton, T., Moewes, A., Finkelstein, L. D., Katsnelson, M. I., Davydov, V. A., Rakhmanina, A. V., Makarova, T. L., Kopelevich, Y., Chiuzbaian, S., and Neumann, M.

We present band structure calculations of rhombohedral C-60 performed in the local-spin-density approximation. Rhombohedral C-60(Rh-C-60) is a two-dimensional polymer of C-60 with trigonal topology. No magnetic solution exists for Rh-C-60 and energy bands with different spins are found to be identical and not split. The calculated C 2p partial density of states is compared to carbon K-edge x-ray emission and absorption spectra and shows good agreement. It is concluded that the rhombohedral distortion of C-60 itself cannot induce magnetic ordering in the molecular carbon. The result of magnetization measurements performed on the same Rh-C-60 sample corroborates this conclusion.

***Physical Review B* 69[11]. 2004.**

P 092- 04 "The effect of arc velocity on cold electrode erosion".

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

Results of experimental investigations of copper cathode erosion in a magnetically driven arc versus arc rotation velocity v are presented. The erosion rate measurements were carried out with the arc burning in air, for magnetic induction values B in the range of 0.005-0.386 T, axial air gas velocity of 7.65 ms(-1), and current of 292 A. It is shown that in the range of small values of v and B, the mass erosion rate diminishes with v and B. Then, the erosion remains constant for a certain range of v and B, and, subsequently, begins to grow. This information is very important for the correct use of magnetic fields to decrease erosion in arc heaters.

***Physics of Plasmas* 11[3], 1214-1219. 2004.**

P 093- 04 "The effect of helical magnetoelastic anisotropy on magnetoimpedance and its second harmonic component in amorphous wires".
Duque, J. G. S., Gomez-Polo, C., Yelon, A., Ciureanu, P., de Araujo, A. E. P., and Knobel, M.

The frequency dependence of the magnetoimpedance of an amorphous magnetic wire displays a behavior that appears to be ferromagnetic resonance, at a frequency of about 900 kHz. A helical anisotropy is induced in this wire by applying a torsional strain. The second harmonic component of the magnetoimpedance signal is also investigated. The reinforcement of this component by the helical magnetoelastic anisotropy is analyzed in terms of the asymmetry in coercivity of the circumferential hysteresis loops of the wire. (C) 2003 Elsevier B.V. All rights reserved.
***Journal of Magnetism and Magnetic Materials* 271[2-3], 390-395. 2004.**

P 094- 04 "Theoretical study of the formation, evolution, and breaking of gold nanowires".
da Silva, E. Z., Novaes, F. D., da Silva, A. J. R., and Fazzio, A

Real time imaging experiments with metal nanowires (NWs), in particular gold under stress, that show their formation, evolution, and breaking, were obtained with high resolution electron microscopy. In order to understand these results, we use density functional theory (DFT) based methods to simulate the evolution of Au NWs. First we use a tight-binding molecular dynamics (TBMD) method to understand the mechanisms of formation of very thin gold NWs. We present realistic simulations for the breaking of these NWs, whose main features are very similar to the experimental results. We show how defects lead to the formation of one-atom constrictions in the Au NW, which evolves into a one-atom-thick necklace chain. Similarly to the experimental results, we obtain that these necklaces can get as long as five-atoms from apex to apex. Before breaking, we obtain relatively large Au-Au bond distances, of the order of 3.0-3.1 Angstrom. A further pull of the wire causes a sudden increase of one of the bond distances, indicating the breaking of the NW. To get some more insight into the electronic structure aspects of this problem, we considered several of our tight-binding structures before breaking and studied them in detail using an ab initio method based on the DFT. By pulling the wire quasi-statically in this case, we also observed the breaking of the wire at similar distances as in the TBMD. This result was independent of the exchange-correlation potential used-either the local density approximation (LDA) or the generalized gradient approximation (GGA). The pulling force before rupture was obtained as 2.4 nN for the LDA, and 1.9 nN for the GGA. Finally, we also present a detailed analysis of the electronic structure properties for the Au neck atoms, such as the density of states and charge densities, for some configurations before the rupture
***Physical Review B* 69[11]. 2004.**

P 095- 04 "Transport of matter and energy in a mesoscopic thermo-hydrodynamic approach".

Madureira, J. R.

We derive a thermo-hydrodynamic theory for particles and energy flow, based on a nonequilibrium grand-canonical ensemble formalism. The time-dependent kinetic coefficients are explicitly given in terms of microscopic mechanical quantities. The time evolution equations describing the coupled flow of energy and particles are derived. The second-rank tensorial fluxes of current of energy and particles present in the nonequilibrium ensemble are nondiagonal. We obtain a generalized Fick's Law, which presents the effect of the energy flow on the particle diffusion equation. (C) 2004 American Institute of Physics.

***Journal of Chemical Physics* 120[16], 7526-7531. 2004.**

P 096- 04 Quantum linear mutual information and classical correlations in globally pure bipartite systems.

R.M. Angelo, S. A. Vitiello, M.A.M. de Aguiar and K. Furuya

We investigate the correlations of initially separable probability distributions in a globally pure bipartite system with two degrees of freedom for classical and quantum systems. A classical version of the quantum linear mutual information is introduced and the two quantities are compared for a system of oscillators coupled with both linear and non-linear interactions. The classical correlations help to understand how much of the quantum loss of purity are due to intrinsic quantum effects and how much is related to the probabilistic character of the initial states, a characteristic shared by both the classical and quantum pictures. Our examples show that, for initially localized Gaussian states, the classical statistical mutual linear entropy follows its quantum counterpart for short times. For non-Gaussian states the behavior of the classical and quantum measures of information are still qualitatively similar, although the fingerprints of the non-classical nature of the initial state can be observed in their different amplitudes of oscillation.

Physica A: Statistical Mechanics and its Applications
Article: Published online via ScienceDirect
http://authors.elsevier.com/sd/article/S0378437104002985

Abstracta

Instituto de Física
Diretor: Prof. Dr. Daniel Pereira
Universidade Estadual de Campinas - UNICAMP
Cidade Universitária C.P. 6165
CEP: 13081-970 - Campinas - SP - Brasil
e-mail: secdir@ifi.unicamp.br

Fone: 0XX 19 3788-5300 / Fax: 0XX 19 3788-3127

Publicação

Biblioteca do Instituto de Física Gleb Wataghin
http://www.ifi.unicamp.br/bif
Diretora Técnica: Rita Aparecida Sponchiado

Elaboração
Tânia Macedo Folegatti
abstract@ifi.unicamp.br

Projeto Gráfico
IgneaDesign

Impressão
Gráfica Central - Unicamp