# Abstracta

Ano XIV - N. 02

**Abr-10** 



**Trabalhos Publicados** 

Março 2010 à Abril 2010

P057-10 à P090 -10

## **Trabalhos Publicados**

[P057-10] "A Contribution to the Estimation of Binary Halide and Pseudo-Halide Equilibrium Constants using a Linear Extrapolation Methodology"

Silva, A. F. D., Ortega, M. M., Melios, C. B., Pezza, L., de Moraes, M., Tenan, M. A., and Oliveira, A. F.

The molar single ion activity coefficient (y(F)) of fluoride ions was determined at 25 degrees C and ionic strengths between 0.100 and 3.00 mol L-1 NaClO4 using an ion-selective electrode. The activity coefficient dependency on ionic strength was determined to be Phi(F) = log y(F) = 0.2315I-0.041I(2). The function Phi(F)(I), combined with functions obtained in previous work for copper (Phi(Cu)) and hydrogen (Phi(H)), allowed us to make the estimation of the stoichiometric and thermodynamic protonation constants of some halides and pseudo-halides as well as the formation constants of some pseudo-halides and fluoride 1:1 bivalent cation complexes. The calculation procedure proposed in this paper is consistent with critically-selected experimental data. It was demonstrated that it is possible to use Phi(F)(I) for predicting the thermodynamic equilibrium parameters independently of Pearson's hardness of acids and bases

Journal of the Brazilian Chemical Society 21[1], 135-U58. 2010.

[P058-10] "A study of the effect of molecular and aerosol conditions in the atmosphere on air fluorescence measurements at the Pierre Auger Observatory"

Abraham, J., Abreu, P., Aglietta, M., Aguirre, C., Ahn, E. J., Allard, D., et all

The air fluorescence detector of the Pierre Auger Observatory is designed to perforin calorimetric measurements of extensive air showers created by Cosmic rays of above 10(18) eV. To correct these measurements for the effects introduced by atmospheric fluctuations, the Observatory contains a group Of monitoring instruments to record atmospheric conditions across the detector site, ail area exceeding 3000 km(2). The atmospheric data are used extensively in the reconstruction of air showers, and are particularly important for the correct determination of shower energies and the depths of shower maxima. This paper contains a summary of the molecular and aerosol conditions measured at the Pierre Auger Observatory since the start of regular operations in 2004, and includes a discussion of the impact of these measurements oil air shower reconstructions. Between 10(18) and 10(20) eV, the systematic Uncertainties due to all atmospheric effects increase from 4% to 8% in measurements of shower energy, and 4 g cm(-2) to 8 g cm(-2) in measurements of the shower maximum. (C) 2010 Elsevier B.V. All rights reserved

Astroparticle Physics 33[2], 108-129. 2010.

[P059-10] "Aharonov-Bohm Interference in Neutral Excitons: Effects of Built-In Electric Fields"

Teodoro, M. D., Campo, V. L., Lopez-Richard, V., Marega, E., Marques, G. E., Gobato, Y. G., Iikawa, F., Brasil, M. J. S. P., AbuWaar, Z. Y., Dorogan, V. G., Mazur, Y. I., Benamara, M., and Salamo, G. J.

We report a comprehensive discussion of quantum interference effects due to the finite structure of neutral excitons in quantum rings and their first experimental corroboration observed in the optical recombinations. The signatures of builtin electric fields and temperature on quantum interference are demonstrated by theoretical models that describe the modulation of the interference pattern and confirmed by complementary experimental procedures

Physical Review Letters 104[8].086401. 2010.

[P060-10] "Analysis and optimization of an all-fiber device based on photonic crystal fiber with integrated electrodes"

Chesini, G., Serrao, V. A., Franco, M. A. R., and Cordeiro, C. M. B.

We present both numerical and experimental studies of an all-fiber device based on the integration of metallic electrodes into photonic crystal fibers (PCF). The device operation consists on applying electrical current to the electrodes which, by Joule effect, expand and squeeze the PCF microstructure in a preferential direction, altering both phase and group birefringence. We investigate the effect of integrating electrodes into the fiber and the dependence of the device sensitivity on the electrode configuration and composition. (C) 2010 Optical Society of America

Optics Express 18[3], 2842-2848. 2010.

[P061-10] "Broadband second harmonic generation of an optical frequency comb produced by four-wave mixing in highly nonlinear fibers"

Cruz, F. C., Marconi, J. D., Cerqueira, A., and Fragnito, H. L.

We demonstrate broadband second harmonic generation of low-energy pulses produced by injecting two single-frequency lasers into a highly nonlinear fiber. Full nonlinear conversion of the corresponding spectra, consisting of broadband (similar to 200 nm) optical frequency combs at similar to 1580 nm, were obtained by using conventional birefringence phase-matching in two BIBO crystals (2-mm and 100-mu m long) with a normal incidence configuration. The crystals were not tilted and the pulses were not compressed. This broadband conversion results from the large phase-matching bandwidth of the nonlinear BIBO crystals at similar to 1550 nm, but also seems to be a consequence of a fundamental comb with small spectral phase variation. (C) 2009 Elsevier B.V. All rights reserved

Optics Communications 283[7], 1459-1462. 2010.

[P062-10] "Collision-Dependent Atom Tunneling Rate - Bose-Einstein Condensates in Double and Multiple Well Traps"

De Oliveira, M. C. and Da Cunha, B. R.

The overlap of localized wave functions in a two-mode approximation leads to interaction (cross-collision) between ultra-cold atoms trapped in distinct sites of a double-well potential. We show that this interaction can significantly change the atom tunneling rate for special trap configurations resulting in an effective linear Rabi regime of population oscillation between the trap wells. In this sense, we demonstrate that cross-collisional effects can significantly extend the validity of the two-mode model approach allowing it to be alternatively employed to explain the recently observed increase of tunneling rates due to nonlinear interactions. Moreover, we investigate the extension for ultra-cold atoms trapped in an optical lattice. Control over the cross-collisional terms, obtained through manipulation of the optical trapping potential, can be used as an engineering tool to study manybody physics

International Journal of Modern Physics B 23[32], 5867-5880. 2009.

[P063-10] "Dislocation Mobility in a Quantum Crystal: The Case of Solid He-4"

Pessoa, R., Vitiello, S. A., and de Koning, M.

We investigate the structure and mobility of dislocations in hcp He-4 crystals. In addition to fully characterizing the five elastic constants of this system, we obtain direct insight into dislocation core structures on the basal plane, which demonstrates a tendency toward dissociation into partial dislocations. Moreover, our results suggest that intrinsic lattice resistance is an essential factor in the mobility of these dislocations. This insight sheds new light on the possible correlation between dislocation mobility and the observed macroscopic behavior of crystalline He-4

Physical Review Letters 104[8]. 085301. 2010.

[P064-10] "Experimental Evidence for the Influence of Mn3+ Concentration on the Impurity Incorporation and Habit Modification Mechanism of Potassium Dihydrogen Phosphate"

Remedios, C. M. R., dos Santos, A. O., Lai, X., Roberts, K. J., Moreira, S. G. C., Miranda, M. A. R., de Menezes, A. S., Rouxinol, F. P., and Cardoso, L. P.

High resolution X-ray diffraction is applied to study Mn3+ doped potassium dihydrogen phosphate (KDP) single crystals as it function of dopant concentration with quantitative dopant composition within the crystals being assessed using Rutherford backscattering spectroscopy (RBS). Synchrotron radiation high resolution X-ray multiple diffraction Studies using both the Renninger scanning and two-dimensional angular mapping techniques are consistent with the Mn3+ ionic complex entering the crystal lattice via a substitutional incorporation mechanism for Mn3+ at a concentration of 0.1 wt %. For a higher Mn concentration of 0.9 wt %, the data indicate incorporation via an interstitial mechanism associated with a decrease in lattice perfection (an increased mosaic spread). This analysis is supported through X-ray powder diffraction studies which reveal lattice contraction for lower dopant levels with lattice dilation for the higher dopant levels. The potential impact of this observation on the associated crystal growth habit modification process is discussed

### Crystal Growth & Design 10[3], 1053-1058. 2010.

# [P065-10] "Impedance and initial magnetic permeability of gadolinium"

Fraga, G. L. F., Pureur, P., and Cardoso, L. P.

In the present work we report on measurements of the complex impedance and the magnetoimpedance of a textured sample of gadolinium metal. The preferential c -axis orientation of the Gd hexagonal structure is perpendicular to the long axis of the sample. From the experimental data, the complex initial magnetic permeability, mu = mu' + i mu'', was obtained as a function of temperature and frequency of the ac exciting

current. We have found that the results for mu'(T) below the spin reorientation temperature may be described as a power law of the reduced temperature t = 1-T/T-SR, where T-SR is the spin reorientation temperature. This behavior suggests that a genuine phase transition occurs at T-SR. Although the impedance displays a weak anomaly at the Curie temperature, T-C, magnetic measurements indicate that the ferromagnetic response of Gd extends up to this critical point. Thus, two different phases characterizes the cooperative magnetic state of this metal. The frequency dependent results for mu' and mu '' were fitted to a modified Debye formula and the obtained parameters allow us to discriminate between the contributions from domain-wall motion and from magnetization rotation. We obtain that the dynamical properties of the domain walls in Gd are governed by a broad distribution of frequencies whose average value diverge at T-SR. The isothermal magnetoimpedance measurements in temperatures smaller than T-SR show an interesting plateau at low dc applied fields. This plateau is limited by a characteristic field H-K whose magnitude decreases rapidly to nearly zero at T-SR, giving further support for the phase transition scenario at this temperature. (C) 2010 American Institute of Physics. [doi:10.1063/1.3288696]

Journal of Applied Physics 107[5]. 053090. 2010.

### [P066-10] "lons at the Water-Vapor Interface"

Tamashiro, M. N. and Constantino, M. A.

We obtain the electrostatic free energy of finite-sized ions near a dielectric interface within the framework of the classical continuum dielectric theory. The ion is modeled as a dielectric sphere with a fixed Uniform Surface charge density. In order to avoid file generation of additional induced charges oil the ionic Surface, it is assumed there is no dielectric contrast between the ion core and the external dielectric medium where it is embedded, which allows in exact Solution of the electrostatic problem by the image-charge method. It is shown that earlier results reported in the literature, especially when there is partial ionic penetration into the interface, always Underestimate the electrostatic free energy associated with nonpolarizable ions. For ail ion modeled as a vacuum cavity at the water-vapor interface, it is estimated that the free energy is ail order of magnitude larger than prior predictions

Journal of Physical Chemistry B 114[10], 3583-3591. 2010.

[P067-10] "Low energy scattering of positrons by H2O"

Arretche, F., Tenfen, W., Mazon, K. T., Michelin, S. E., Lima, M. A. P., Lee, M. T., Machado, L. E., Fujimoto, M. M., and Pessoa, O. A.

We present a theoretical investigation on elastic positron-H2O collisions. More specifically, differential and integral cross sections in the 0-10 eV energy range are reported. The calculations were performed using two theoretical approaches, namely, the Schwinger multichannel method and the method of continued fractions. The positron-molecule interaction dynamics is described by using a potential composed of static and correlation-polarization contributions. Comparison of our calculated results with the recent experimental of Zecca et al. [J. Phys. B 39 (2006) 1597] and theoretical results is encouraging. (C) 2009 Elsevier B.V. All rights reserved

Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms 268[2], 178-182. 2010.

# [P068-10] "Magnon anomalous interactions from SU(2) gauge symmetry: Are magnons 'charged' under spin?"

Dartora, C. A. and Cabrera, G. G.

The Pauli-Schrodinger non-relativistic theory of spin-1/2 charged fermions requires invariance under the  $U(1) \times SU(2)$  gauge group. The U(1) symmetry responds for the usual coupling of a charged particle to the electromagnetic gauge potentials A(mu), while the spin interactions with the electromagnetic fields are obtained by changing the status of the global SU(2) rotational invariance of the Pauli-Schrodinger Lagrangian density to a local SU(2) gauge symmetry, for which the electric and magnetic fields E and B play the role of gauge potentials. Assuming that local gauge invariance under rotations can be applied to an arbitrary spin-S quantum field we extend the SU(2) gauge symmetry to the magnon field theory of Heisenberg ferromagnets. It is shown that the magnon field couples to the corresponding gauge fields, E and B, yielding 'anomalous' interactions of magnons with the electric component of the electromagnetic field, as in the case of charged excitations. (C) 2009 Elsevier B.V. All rights reserved

Physica B-Condensed Matter 405[4], 1158-1162. 2010.

[P069-10] "Measurement of the Depth of Maximum of Extensive Air Showers above 10(18) eV"

Abraham, J., Abreu, P., Aglietta, M., Ahn, E. J., Allard, D., Allekotte, I., Allen, J., et all

We describe the measurement of the depth of maximum, X-max, of the longitudinal development of air showers induced by cosmic rays. Almost 4000 events above 10(18) eV observed by the fluorescence detector of the Pierre Auger Observatory in coincidence with at least one surface detector station are selected for the analysis. The average shower maximum was found to evolve with energy at a rate of (106 +/- 35-21) g/cm(2)/decade below 10(18.24) +/- (0.05) eV, and d24 +/- 3 g/cm(2)/ecade above this energy. The measured shower-to-shower fluctuations decrease from about 55 to 26 g/cm(2). The interpretation of these results in terms of the cosmic ray mass composition is briefly discussed

Physical Review Letters 104[9]. 091101. 2010.

[P070-10] "Measurement of the energy spectrum of cosmic rays above 10(18) eV using the Pierre Auger Observatory"

Abraham, J., Abreu, P., Aglietta, M., Ahn, E. J., Allard, D., Allen, J., et all

We report a measurement of the flux of cosmic rays with unprecedented precision and Statistics using the Pierre Auger Observatory Based on fluorescence observations in coincidence with at least one Surface detector we derive a spectrum for energies above 10(18) eV We also update the previously published energy spectrum obtained with the surface detector array The two spectra are combined addressing the systematic uncertainties and, in particular. the influence of the energy resolution on the spectral shape The spectrum can be described by a broken power law E-gamma with index gamma = 3 3 below the ankle which is measured at log(10)(E-ankle/eV) = 18 6 Above the ankle the spectrum is described by a power law with index 2 6 followed by a flux suppression, above about log(10)(E/eV) = 19 5, detected with high statistical significance (C) 2010 Elsevier B V All rights reserved

Physics Letters B 685[4-5], 239-246. 2010.

### [P071-10] "MMP-2 Regulates Rat Ventral Prostate Development In Vitro"

Bruni-Cardoso, A., Rosa-Ribeiro, R., Pascoal, V. D. B., De Thomaz, A. A., Cesar, C. L., and Carvalho, H. F.

We have hypothesized that epithelial growth, branching, and canalization in the rodent ventral prostate (VP) would require matrix remodeling, and hence matrix metalloproteinase (MMP) activity. Therefore, the aim of this study was to evaluate the impact of blocking MMP-2, using whole organ culture. siRNA was employed to inhibit MMP-2 expression, and this was compared to GM6001's (a broad-spectrum MMP inhibitor) inhibition of general MMPs. These blocks impaired VP morphogenesis. MMP-2 silencing reduced organ size, epithelial area, and the number of tips, as well as caused a dilation of the distal parts of the epithelium. Histology, 3-D reconstruction, biochemistry, and second harmonic generation (SHG) revealed that MMP-2 silencing affected VP architecture by interfering in epithelial cell proliferation, lumen formation, and cellular organization of both epithelium and stroma, besides intense accumulation of collagen fibers. These data suggest that MMP-2 plays important roles in prostate growth, being directly involved with epithelial morphogenesis. Developmental Dynamics 239:737-746, 2010. (C) 2010 Wiley-Liss, Inc

Developmental Dynamics 239[3], 737-746. 2010.

[P072-10] "Nanoparticle Platform to Modulate Reaction Mechanism of Phenothiazine Photosensitizers"

Tada, D. B., Rossi, L. M., Leite, C. A. P., Itri, R., and Baptista, M. S.

Herein, we report on the synthesis of photosensitizing nanoparticles in which the generation of different oxidizing species, i.e., singlet oxygen (0-1(2)) or radicals, was modulated. Sol gel and surface chemistry were used to obtain nanoparticles with specific ratios of dimer to monomer species of phenothiazine photosensitizers (PSs). Due to competition between the reactions involving electron transfer within dimer species and energy transfer from monomer triplets to oxygen, the efficiency of O-1(2) generation could be controlled. Nanoparticles with an excess of dimer have an O-1(2) generation efficiency (S-Delta) of 0.01 while those without dimer have a S, value of 0.4. Furthermore, we demonstrate that the PS properties of the nanoparticles are not subjected to interference from the external medium as is commonly the case for free PSs, i.e., PS ground and triplet states are not reduced by NADH and ascorbate, respectively, and singlet excited states are less suppressed by bromide. The modulated O-1(2) generation and the PS protection from external interferences make this nanoparticle platform a promising tool to aid in performing mechanistic studies in biological systems. Also, it offers potential application in technological areas in which photo-induced processes take place

Journal of Nanoscience and Nanotechnology 10[5], 3100-3108. 2010.

[P073-10] "Observation of an Antimatter Hypernucleus"

Abelev, B. I., Aggarwal, M. M., Ahammed, Z., Alakhverdyants, A. V., Alekseev, I., et all

We report on the first experimental evidence of a Schottky barrier effect produced by the action of light in an otherwise purely Ohmic contact between a nominally undoped photorefractive titanosillenite Bi12TiO20 crystal and a transparent conductive SnO2 electrode. The photorefractive crystal is sandwiched between two transparent electrodes and a Schottky barrier is built up in the illuminated crystal-electrode interface under the action of light with photonic energy large enough to excite charge carriers from the Fermi level into the conduction band. The contact remains purely Ohmic under illumination with photonic energy below that of the Fermi gap and the photoinduced barrier almost disappears if the photonic energy is large enough to produce electron-hole pairs

Physical Review Letters 104[11]. 116601. 2010.

[P074-10] "Photoinduced Schottky Barrier in Photorefractive Materials"

Frejlich, J., Longeaud, C., and Carvalho, J. F.

We report on the first experimental evidence of a Schottky barrier effect produced by the action of light in an otherwise purely Ohmic contact between a nominally undoped photorefractive titanosillenite Bi12TiO20 crystal and a transparent conductive SnO2 electrode. The photorefractive crystal is sandwiched between two transparent electrodes and a Schottky barrier is built up in the illuminated crystal-electrode interface under the action of light with photonic energy large enough to excite charge carriers from the Fermi level into the conduction band. The contact remains purely Ohmic under illumination with photonic energy below that of the Fermi gap and the photoinduced barrier almost disappears if the photonic energy is large enough to produce electron-hole pairs

Physical Review Letters 104[11]. 116601. 2010.

[P075-10] "Physical Properties of Water Near a Gold Surface: A Nanorheological Analysis"

Soares, D. M., Tenan, M. A., Gomide, A. B., and Gomes, W. E.

Water at room temperature is not simply a medium for which uniform properties can always be assumed. Water close to solid hydrophobic or hydrophilic surfaces has elasticity, which is measured by monitoring the quartz crystal microbalance (QCM) resonant frequency and resistance. Small additions of salt are shown to modify this elasticity. Furthermore, near the hydrophobic QCM gold electrode, undersaturated aqueous NaCl solutions present a high concentration of ion pairs, which is confirmed by atomic force microscopy through force versus distance measurements

Chemphyschem 11[4], 905-911. 2010.

[P076-10] "Poly(n-alkylsilsesquioxane)s: Synthesis, Characterization, and Modification with Poly(dimethylsiloxane)"

De Prado, L. A. S. A., Torriani, I. L., and Yoshida, I. V. P.

Self-supported translucent films constituted of poly(noctylsilsesquioxane) or poly(n-dodecylsilsesquioxane) were obtained from the hydrolysis and condensation of n-octyltriethoxysilane (OTES) or n-dodecyltriethoxysi lane (DTES), respectively. Dense films were obtained in the absence of organic solvents, with dibutyltin diacetate as catalyst.

These films exhibited good optical transparency and thermal stability. The incorporation of oligomeric dimethylsiloxane units (D-Me, D-Me) in these materials, derived from silanol-terminated poly(dimethylsiloxane) (PDMS) or 1,1,3,3-tetramethyl-1,3diethoxydisiloxane (TMDES), was carried out during the hydrolysis and condensation of OTES and DTES and was confirmed by solidstate Si-29 NMR. Poly(n-octylsilsesquioxane) showed a glasstransition temperature at -65 degrees C, due to the increase in the free volume, promoted by the bulky n-octyl groups. The differential scanning calorimetric (DSC) curves of the polymer derived from DTES were characterized by first-order transitions at temperatures ranging from -15.8 to -0.7 degrees C. Further studies of these networks by low-temperature XRD evidenced narrowing of the diffraction halos suggesting a partial order-disorder transition for these materials at lower temperatures. Good thermal stability up to 350 degrees C and the solvent-free production process make these polymers potential candidates for the development of self-supported hydrophobic protective coatings. (C) 2010 Wiley Periodicals, Inc. J Polym Sci Part A: Polym Chem 48: 1220-1229, 2010

Journal of Polymer Science Part A-Polymer Chemistry 48[5], 1220-1229. 2010.

[P077-10] "Solving the thermal stability problem at the HfO2/ Si interface with previous N implantation"

Carazzolle, M. F., Fluchter, C. R., de Siervo, A., Pancotti, A., Weier, D., Schurmann, M., Westphal, C., Landers, R., and Kleiman, G. G.

We report on the use of N implantation to produce thin, pure, uniform, and thermally stable Si3N4 buffer layers and HfO2 overlayers on Si(100) and Si(111) without silicide formation. (C) 2010 American Institute of Physics. [doi: 10.1063/1.3298438]

Journal of Applied Physics 107[5]. 056010. 2010.

[P078-10] "Specific heat of Gd4Co3"

Seixas, T. M., da Silva, M. A. S., de Lima, O. F., Lopez, J., Braun, H. F., and Eska, G.

The specific heat (C(T)) of Gd4Co3 was measured in the temperature range 2-300 K and its magnetic contribution (C-m(T))was determined using a new method that fits the electronic specific heat coefficient (gamma) and the Debye temperature (theta(D)) by constraining the resulting magnetic entropy (S-m(T))to saturate at temperatures far above the Curie temperature (T-C). C-m(T) exhibits a low-temperature bump originating from thermal excitation of gapped spin waves, which is responsible for pronounced peaks, at approximate to 35 K, in both C-m/T and the temperature derivative of the magnetic contribution to electrical resistivity (d rho(m)/dT). Apart from in the vicinity of T-C, an excellent global correlation was found between C-m/T and d rho(m)/dT. Our results provide strong support for the consistency of the new method proposed for the determination of C-m(T) and rule out any major role of short-range order on Gd moments or d-electron spin fluctuation effects in the paramagnetic phase. A comparative analysis with other methods used in similar compounds points to the need for a better evaluation of C-m(T)in such compounds, especially in the magnetically ordered phase, where a deficient evaluation of C-m/T has a larger impact on the S-m(T) curve

Journal of Physics-Condensed Matter 22[13]. 136002. 2010.

[P079-10] "System-reservoir dynamics of quantum and classical correlations"

Maziero, J., Werlang, T., Fanchini, F. F., Celeri, L. C., and Serra, R. M.

We examine the system-reservoir dynamics of classical and quantum correlations in the decoherence phenomenon within a two-qubit composite system interacting with two independent environments. The most common noise channels (amplitude damping, phase damping, bit flip, bit-phase flip, and phase flip) are analyzed. By analytical and numerical analyses we find that, contrary to what is usually stated in the literature, decoherence may occur without entanglement between the system and the environment. We also show that, in some cases, the bipartite quantum correlation initially present in the system is completely evaporated and not transferred to the environments

Physical Review A 81[2].022116. 2010.

[P080-10] "System size dependence of associated yields in hadron-triggered jets STAR Collaboration"

Abelev, B. I., Aggarwal, M. M., Ahammed, Z., Anderson, B. D., Arkhipkin, D., et all

We present results on the system size dependence of high transverse momentum di-hadron correlations at root s(NN) = 200 GeV as measured by STAR at RHIC. Measurements in d + Au, Cu + Cu and Au + Au collisions reveal similar jet-like near-side correlation yields (correlations at small angular separation Delta phi similar to 0, Delta eta similar to 0) for all systems and centralities. Previous measurements have shown Chat the away-side (Delta phi similar to pi) yield is suppressed in heavy-ion collisions. We present measurements of the away-side Suppression as a function of transverse momentum and centrality in Cu + Cu and Au + Au collisions. The suppression is found to be similar in Cu + Cu and An + An collisions at a similar number of participants. The results are compared to theoretical calculations based on the patron guenching model and the modified fragmentation model. The observed differences between data and theory indicate that the correlated yields presented here will further constrain dynamic energy loss models and provide information about the dynamic density profile in heavy-ion collisions. (C) 2009 Elsevier B.V. All rights reserved

Physics Letters B 683[2-3], 123-128. 2010.

[P081-10] "The Role of Nonequilibrium Thermo-Mechanical Statistics in Modern Technologies and Industrial Processes: An Overview"

Rodrigues, C. G., Silva, A. A. P., Silva, C. A. B., Vasconcellos, A. R., Ramos, J. G., and Luzzi, R.

The nowadays notable development of all the modern technology, fundamental for the progress and well being of world society, imposes a great deal of stress in the realm of basic Physics, more precisely on Thermo-Statistics. We do face situations in electronics and optoelectronics involving physical-chemical systems far-removed-from equilibrium, where ultrafast (in pico- and femto-second scale) and non-linear processes are present. Further, we need to be aware of the rapid unfolding of nano-technologies and use of low-dimensional systems (e.g., nanometric quantum wells and quantum dots in semiconductor heterostructures). All together this demands having an access to a Statistical Mechanics being efficient to deal with such requirements. It is worth noticing that the renowned Ryogo Kubo once stated that "statistical mechanics has been considered a theoretical endeavor. However, statistical mechanics exists for the sake of the real world, not for fictions. Further progress can only be hoped by close cooperation with experiment". Moreover, one needs to face the study of soft matter and fluids with complex structures (usually of the average self-affine fractal-like type). This is relevant for technological improvement in industries like, for example, that of polymers, petroleum, cosmetics, food, electronics and photonics (conducting polymers and glasses), in medical engineering, etc. It is then required to introduce a thermo-hydrodynamics going well beyond the classical (Onsagerian) one. Moreover, in the both type of situations above mentioned there often appear difficulties of description and objectivity (existence of so-called "hidden constraints"), which impair the proper application of the conventional ensemble approach used in the general, logically and physically sound, and well established Boltzmann-Gibbs statistics. A tentative to partially overcome such difficulties consists in resorting to non-conventional approaches. Here we briefly describe the construction of a Non-Equilibrium Statistical Ensemble Formalism (NESEF) that can deal, within a certain degree of success, with the situations above described. Several particular instances involving experimental observations and measurements in the area of semiconductor physics and in physics of fluids, which were analyzed in the context of the theory, are summarized. They comprise the cases of ultrafast optical spectroscopy; optical and transport processes in lowdimensional complex semiconductors; nonlinear transport in doped highly-polar semiconductors (of use in "blue diodes") under moderate to high electric fields; nonlinear higher-order thermohydrodynamics in fluids under driven flow, in normal solutions and in complex situations as in solutions of polymers, micelles, DNA, and in microbatteries

### Brazilian Journal of Physics 40[1], 63-91. 2010.

[P082-10] "Theoretical study of the heteroepitaxial growth of Pd on Cu(111), Pd on Ni(111), Ni on Pd(111), and Cu on Pd(111) using a semiempirical method"

Negreiros, F. R., Soares, E. A., de Siervo, A., Paniago, R., de Carvalho, V. E., and Landers, R.

Heteroepitaxy has been widely studied by many different theoretical and experimental techniques. Each technique focuses on some features of the growth process, and only by combining the information each provides a full characterization can be given. In this work, the growth of Pd on Ni (111), Pd on Cu (111), Cu on Pd (111), and Ni on Pd (111) is studied with a purely energetic approach which consists of determining a unit cell with a size that depends on the relation between the lateral misfit of the deposited film and the substrate. The energetic is evaluated using a semiempirical coupled with a genetic algorithm global search method to determine with accuracy the relaxation magnitudes of the system. With this approach, features such as interlayer spacings, variation in the film's lattice parameter with coverage, and diffusion influence in the growth process are studied qualitative and guantitatively. The results obtained are directly compared with experimental findings from literature and also presented in this work. The theory-experiment comparison shows that the methodology used is successful in describing qualitatively most features of all four systems. However, for the Pd on Cu (111) case, poor agreement is found, and the analysis of the influence of diffusion and temperature suggests that a somewhat complex alloy formation in the interface is expected for this particular system

Physical Review B 81[8]. 085437. 2010.

[P083-10] "Thermo-Statistical Theory of Kinetic and Relaxation Processes"

Vannucchi, F. S., Vasconcellos, A. R., and Luzzi, R.

We describe, in a short overview, the construction of a Non equilibrium Statistical Mechanics Ensemble Formalism, providing a thermo-statistical theory of kinetic and relaxation processes. Such construction has been approached along the recently past 20th century by a pleiad of distinguished scientists, a work that can be subsumed in a large systematization in the form of a physically sound, general and useful, theoretical framework. We briefly comment on the main guestions associated to that construction. Among them are the relevant ones of choice of the basic variables, and of historicity and irreversibility. The derivation of an on equilibrium grand-canonical statistical operator and a brief description of the all-important accompanying Nonlinear Quantum Kinetic Theory of relaxation processes are presented. The a spect of validation of the theory (comparison of theory and experiment) is reviewed in compact form, and its use is illustrated in a study of a nonequilibrium system of quantum oscillators embedded in a thermal bath and under the action of an external force, showing how a far-reaching generalization of Mori-Langev in equations arises

International Journal of Modern Physics B 23[27], 5283-5305. 2009.

[P084-10] "Thermodynamic Simulation of Biomass Gas Steam Reforming for A Solid Oxide Fuel Cell (Sofc) System"

Sordi, A., da Silva, E. P., Neto, A. J. M., Lopes, D. G., Pinto, C. S., and Araujo, P. D.

This paper presents a methodology to simulate a small-scale fuel cell system for power generation using biomass gas as fuel. The methodology encompasses the thermodynamic and electrochemical aspects of a solid oxide fuel cell (SOFC), as well as solves the problem of chemical equilibrium in complex systems. In this case the complex system is the internal reforming of biomass gas to produce hydrogen. The fuel cell input variables are: operational voltage, cell power output, composition of the biomass gas reforming, thermodynamic efficiency, electrochemical efficiency, practical efficiency, the First and Second law efficiencies for the whole system. The chemical compositions, molar flows and temperatures are presented to each point of the system as well as the exergetic efficiency. For a molar water/carbon ratio of 2, the thermodynamic simulation of the biomass gas reforming indicates the maximum hydrogen production at a temperature of 1070 K, which can vary as a function of the biomass gas composition. The comparison with the efficiency of simple gas turbine cycle and regenerative gas turbine cycle shows the superiority of SOFC for the considered electrical power range

Brazilian Journal of Chemical Engineering 26[4], 745-755. 2009.

[P085-10] "Thermophoretically driven carbon nanotube oscillators"

Coluci, V. R., Timoteo, V. S., and Galvao, D. S.

The behavior of a nanodevice based upon double-walled carbon nanotube oscillators driven by periodically applied thermal gradients (7 and 17 K/nm) is investigated by numerical calculations and classical molecular dynamics simulations. Our results indicate that thermophoresis can be effective to initiate the oscillator and that suitable heat pulses may provide an appropriate way to tune its behavior. Sustained regular oscillatory as well as chaotic motions were observed for the systems investigated in this work. (C) 2009 American Institute of Physics. [doi:10.1063/1.3276546]

Applied Physics Letters 95[25]. 253103. 2009.

[P086-10] "Titanium-aluminum oxynitride (TAON) as high-k gate dielectric for sub-32 nm CMOS technology"

Miyoshi, J., Diniz, J. A., Barros, A. D., Doi, I., and Von Zuben, A. A. G.

High-k insulators for the next generation (sub-32 nm CMOS (complementary metal-oxide-semiconductor) technology). such as titanium-aluminum oxynitride (TAON) and titanium-aluminum oxide (TAO), have been obtained by Ti/Al e-beam evaporation, with additional electron cyclotron resonance (ECR) plasma oxynitridation and oxidation on Si substrates, respectively. Physical thickness values between 5.7 and 6.3 nm were determined by ellipsometry. These films were used as gate insulators in MOS capacitors fabricated with Al electrodes, and they were used to obtain capacitance-voltage (C-V) measurements. A relative dielectric constant of 3.9 was adopted to extract the equivalent oxide thickness (EOT) of films from C-V curves under strong accumulation condition, resulting in values between 1.5 and 1.1 nm, and effective charge densities of about 10(11) cm(-2). Because of these results, nMOSFETs with Al gate electrode and TAON gate dielectric were fabricated and characterized by current-voltage (I-V) curves. From these nMOSFETs electrical characteristics, a sub-threshold slope of 80 mV/dec and an EOT of 0.87 nm were obtained. These results indicate that the obtained TAON film is a suitable gate insulator for the next generation (MOS) devices. (C) 2009 Elsevier B.V. All rights reserved

Microelectronic Engineering 87[3], 267-270. 2010.

[P087-10] "Trigger and aperture of the surface detector array of the Pierre Auger Observatory"

Abraham, J., Abreu, P., Aglietta, M., Ahn, E. J., Allard, D., Allekotte, I., Allen, J., et all

The surface detector array of the Pierre Auger Observatory consists of 1600 water-Cherenkov detectors, for the study of extensive air showers (EAS) generated by ultra-high-energy cosmic rays. We describe the trigger hierarchy, from the identification of candidate showers at the level of a single detector, amongst a large background (mainly random single cosmic ray muons), up to the selection of real events and the rejection of random coincidences. Such trigger makes the surface detector array fully efficient for the detection of EAS with energy above 3 x 10(18) eV, for all zenith angles between 0 degrees and 60 degrees, independently of the position of the impact point and of the mass of the primary particle. In these range of energies and angles, the exposure of the surface array can be determined purely on the basis of the geometrical acceptance. (C) 2009 Elsevier B.V. All rights reserved

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment 613[1], 29-39. 2010.

<ul> <li>[P088-10] "Ultrahigh-birefringent squeezed lattice photonic crystal fiber with rotated elliptical air holes"</li> <li>Beltran-Mejia, F., Chesini, G., Silvestre, E., George, A. K., Knight, J. C., and Cordeiro, C. M. B.</li> <li>We report an experimental realization of a highly birefringent photonic crystal fiber as a result of compressing a regular hexagonal structure. The experimental measurements estimate a group birefringence of approximately 5.5 X 10(-3) at 1550 nm in good agreement with the numerical results. We study the influence of compressing the regular structure at different directions and magnifications, obtaining a method to realistically enhance the phase birefringence while moderating the group birefringence. (C) 2010 Optical Society of America</li> <li>Optics Letters 35[4], 544-546. 2010.</li> <li>[P089-10] "Zero-point divacancy concentration in the shadow wave function model for solid He-4"</li> <li>Pessoa, R., de Koning, M., and Vitiello, S. A.</li> <li>We address the issue of interaction between zero-point vacancies in solid He-4 as described within the shadow wave function model.</li> <li>Applying the reversible-work method and taking into account finite-size effects, we obtain a zero-point monovacancy concentration of (2.03 +/- 0.02)x10(-3), which is slightly higher than the result due to Reatto for the same model. Utilizing the same methodology, we then consider the divacancy, taking into account both the in-plane as well as out-of-plane configurations with respect to the basal plane. We find no significant anisotropy between both conformations. Furthermore, although there is a small binding tendency, the expected divacancy concentration is only similar to 4-5 times larger than the value expected in the aground state</li> <li>Physical Review B 80[17]. 172302. 2009.</li> <li>[P090-10] "Zircon fission track and U-Th-Pb in situ dating of Rio Parana Formation, Parana Basin, Brazil"</li> <li>Dias, A. N. C., Tello, C. A., Chemale, F., lunes, P. J., Soares, C. J., Curvo, E. A., Guedes, S.</li></ul>	dating methods. The obtained ages are from same zircon grain that provided information on the source areas for the sediments and the morphotectonic events Revista Mexicana de Fisica 56[1], 16-21. 2010. Adendo da edição anterior do artigo [P049-10] [P049-10] "Stability of a pendulum with periodic arbitrary forcing" Quintero-Cabra, P., Silva-Valencia, J., and Alejo-Martinez, H. The dynamics of a driven pendulum at arbitrary angles and signals is studied using the lagrangian formalism and the effective potential method. We make a general discussion of the problem and consider three particular driving signals: sinusoidal, square and triangular. Was found that the cut off frequency, which determines the transition between the stability and nonstability regions depends on the type of signal used. For square driving the lower bound is minimum, while for the triangular drive is a maximum, the usual case of sinusoidal driving was found between the previous ones. Revista Mexicana de Fisica e 55[2], 161-167. 2009.
<b>Abstracta</b> Instituto de Física Diretor: Prof. Dr. Daniel Pereira Universidade Estadual de Campinas - UNICAMP Cidade Universitária Zeferino Vaz 13083-859 - Campinas - SP - Brasil	Publicação Biblioteca do Instituto de Física Gleb Wataghin http://webbif.ifi.unicamp.br Diretora Técnica: Sandra Maria Carlos Cartaxo Elaboração Antonela Carvalho Ribeiro antonela@ifi.unicamp.br Proieto Gráfico

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