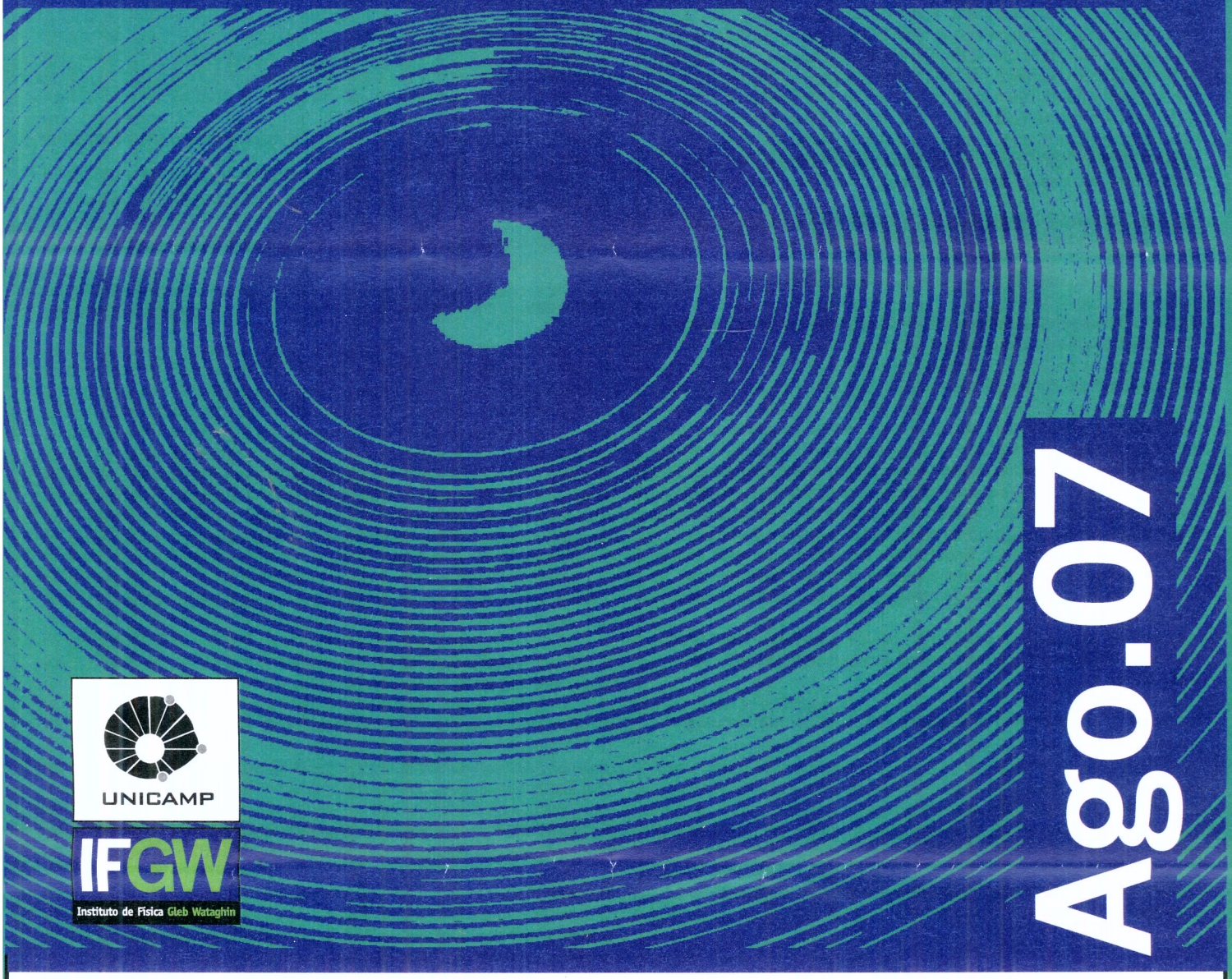
Abstracta

Ano IX- N. 03



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TRABALHOS ACEITOS PARA PUBLICAÇÃO

A 009- 07 Transient transport in III-nitrides: interplay of momentum and energy relaxation times.

TRABALHOS PUBLICADOS

JULHO DE 2007 A AGOSTO DE 2007

P 118-07 à P 174-07

TRABALHOS ACEITOS PARA PUBLICAÇÃO

A 009-07 Transient transport in III-nitrides: interplay of momentum and energy relaxation times

Rodrigues, C. G., Vasconcellos, A. R, Luzzi. L., and Freire, V. N.

The ultrafast transient transport in wide-gap polar III-nitride semiconductors in electric fields is considered. A nonlinear and time-dependent (on the evolution of the nonequilibrium-irreversible thermodynamic state of the system) Drude-like law is derived, with the conductivity related to a so-called transport time (or current characteristic time which is related to a memory-dependent momentum relaxation time). From the collision operators, present in the evolution equations for the carriers' energy and momentum, are obtained quantities playing the role of time-dependent energy and momentum relaxation times. The electron drift velocity overshoot at intermediate-intensity fields in GaN, AlN and InN is evidenced, and its onset is explained as a result of the interplay of momentum and energy relaxation times.

Journal of Physics: Condensed Matter, accepted on July 2007.

TRABALHOS PUBLICADOS

P 118-07 "A semiclassical trace formula for the canonical partition function of one dimensional systems"

Parisio, F. and de Aguiar, M. A. M

We present a semiclassical trace formula for the canonical partition function of arbitrary one-dimensional systems. The approximation is obtained via the stationary exponent method applied to the phase-space integration of the density operator in the coherent state representation. The formalism is valid in the low temperature limit, presenting accurate results in this regime. As illustrations we consider a quartic Hamiltonian that cannot be split into kinetic and potential parts, and a system with two local minima. Applications to spin systems are also presented. (c) 2007 Elsevier B.V. All rights reserved

Physica A-Statistical Mechanics and Its Applications 380, 211-225. 2007.

P 119-07 "Acupuncture for migraine prophylaxis: methodological issues"

Alecrim-Andrade, J., Carne, X., Correa, H. R., Maciel, J. A., Peres, M. F. P., and Vasconcelos, G.M. S.

Cephalalgia 27[6], 754-754. 2007.

P 120-07 "Anisotropy studies around the galactic centre at EeV energies with the Auger Observatory"

Abraham, J., et al...

Data from the Pierre Auger Observatory are analyzed to search for anisotropies near the direction of the Galactic Centre at EeV energies. The exposure of the surface array in this part of the sky is already significantly larger than that of the fore-runner experiments. Our results do not support previous findings of localized excesses in the AGASA and SUGAR data. We set an upper bound on a point-like flux of cosmic rays arriving from the Galactic Centre which excludes several scenarios predicting sources of EeV neutrons from Sagittarius A. Also the events detected simultaneously by the surface and fluorescence detectors (the 'hybrid' data set), which have better pointing accuracy but are less numerous than those of the surface array alone, do not show any significant localized excess from this direction. (c) 2006 Elsevier B.V. All rights reserved

Astroparticle Physics 27[4], 244-253. 2007.

P 121- 07"Charge-separated atmospheric neutrino-induced muons in the MINOS fardetector"

Adamson, P., et al

We found 140 neutrino-induced muons in 854.24 live days in the MINOS far detector, which has an acceptance for neutrino-induced muons of 6.91x10(6) cm(2) sr. We looked for evidence of neutrino disappearance in this data set by computing the ratio of the number of low momentum muons to the sum of the number of high momentum and unknown momentum muons for both data and Monte Carlo expectation in the absence of neutrino oscillations. The ratio of data and Monte Carlo ratios, R, is R=0.65(-0.12)(+0.15)(stat)+/- 0.09(syst), a result that is consistent with an oscillation signal. A fit to the data for the oscillation parameters sin(2)2 theta(23) and Delta m(23)(2) excludes the null oscillation hypothesis at the 94% confidence level. We separated the muons into mu(-) and mu(+) in both the data and Monte Carlo events and found the ratio of the total number of mu(-) to mu(+) in both samples. The ratio of those ratios, R boolean AND(CPT), is a test of CPT conservation. The result R boolean AND(CPT)=0.72(-0.18)(+0.24)(stat)(-0.04)(+0.08)(syst) is consistent with CPT conservation

Physical Review D 75[9]. 2007.

P 122- 07"Detection of resonance space-charge wave peaks for holes and electrons in photorefractive crystals"

de Oliveira, I. and Frejlich, J.

We report nonstationary photorefractive holograms in absorbing Bi-12TiO20 samples with different degrees of hole-electron competition exhibiting resonance peaks due to electron and hole charge carriers. One sample with moderate hole-electron competition and another with a much larger effect were studied. Experimental data from these samples were analyzed using a theoretical model accounting for electrical hole-electron coupling, wave coupling, and response-time variation along the sample thickness due to bulk light absorption. Comparing experimental data and theoretical results allows finding out material parameters adequately describing hole and electron photoactive centers Moreira, W. O., Landers, R., and Kleiman, G. G.

Journal of Electron Spectroscopy and Related Phenomena 156, CIII-CIII. 2007.

P 123- 07"Determination of relative Fermi level in metallic binary alloys (Pd-Au) with Argon implantation"

Moreira, W. O., Landers, R., and Kleiman, G. G.

Journal of Electron Spectroscopy and Related Phenomena 156, CIII-CIII. 2007.

P 124- 07"Dirac neutrino mass from the beta-decay end point modified by the dynamics of a Lorentz-violating equation of motion"

Bernardini, A. E.

Using a generalized procedure for obtaining the equation of motion of a propagating fermionic particle, we examine previous claims for a light-like preferred axis embedded in the framework of Lorentz-invariance violation with preserved algebra. In a high energy scale, the corresponding equation of motion is reduced to a conserving lepton number chiral (very special relativity) equation, and in a low energy scale, the Dirac equation for a free particle is recovered. The new dynamics introduces some novel ingredients (modified cross section) to the phenomenology of the tritium beta-decay end point

Physical Review D 75[9]. 2007.

Trabalhos Publicados

P 125-07 "Effect of breakup on elastic scattering for the Li-6,Li-7+Co-59 systems"

Souza, F. A., Leal, L. A. S., Carlin, N., Munhoz, M. G., Neto, R. L., de Moura, M. M., Suaide, A. A.P., Szanto, E. M., de Toledo, A. S., Takahashi, J., and Takahashi, J.

The elastic scattering for the Li-6,Li-7+Co-59 systems was investigated in the bombarding energy range 12 MeV <= E-lab <= 30 MeV by means of an analysis using the Sao Paulo potential, through which the behavior of the real and imaginary parts as function of the bombarding energy was established. The experimental results suggest that overall there is an evidence of the usual threshold anomaly for both systems, although for the Li-6+Co-59 system, an evidence of the breakup threshold anomaly could also be questioned

Physical Review C 75[4]. 2007.

P 126-07 "Effects in electronic structure of implanted xenon with low energy in amorphous silicon"

Barbieri, P. F. and Marques, F. C.

Journal of Electron Spectroscopy and Related Phenomena 156, XCVII-XCVII. 2007.

P 127-07 "Electron and positron scattering from 1,1-C2H2F2"

Makochekanwa, C., Kato, H., Hoshino, M., Bettega, M. H. F., Lima, M. A. P., Sueoka, O., and Tanaka, H.

1,1-difluoroethylene (1,1-C2H2F2) molecules have been studied for the first time experimentally and theoretically by electron and positron impact. 0.4-1000 eV electron and 0.2-1000 eV positron impact total cross sections (TCSs) were measured using a retarding potential time-of-flight apparatus. In order to probe the resonances observed in the electron TCSs, a crossed-beam method was used to investigate vibrational excitation cross sections over the energy range of 1.3-49 eV and scattering angles 90 degrees and 120 degrees for the two loss energies 0.115 and 0.381 eV corresponding to the dominant C-H (nu(2) and nu(9)) stretching and the combined C-F (nu(3)) stretching and CH2 (nu(11)) rocking vibrations, respectively. Electron impact elastic integral cross sections are also reported for calculations carried out using the Schwinger multichannel method with pseudopotentials for the energy range from 0.5 to 50 eV in the static-exchange approximation and from 0.5 to 20 eV in the static-exchange plus polarization approximation. Resonance peaks observed centered at about 2.3, 6.5, and 16 eV in the TCSs have been shown to be mainly due to the vibrational and elastic channels, and assigned to the B-2, B-1, and A(1) symmetries, respectively. The pi* resonance peak at 1.8 eV in C2H4 is observed shifted to 2.3 eV in 1,1-C2H2F2 and to 2.5 eV in C2F4; a phenomenon attributed to the decreasing C=C bond length from C2H4 to C2F4. For positron impact a conspicuous peak is observed below the positronium formation threshold at about 1 eV, and other less pronounced ones centered at about 5 and 20 eV. (c) 2007 American Institute of Physics

Journal of Chemical Physics 126[16]. 2007.

P 128-07 "Electron collisions with furan"

Bettega, M. H. F. and Lima, M. A. P.

The authors report integral, differential and momentum transfer cross sections for elastic scattering of low-energy electrons by C4H4O (furan) molecules. Their calculations employed the Schwinger multichannel method with pseudopotentials and were performed in the static-exchange and in the static-exchange plus polarization approximations. The authors found two shape resonances located around 2.1 and 4.2 eV that belong to the B-1 and A(2) symmetries of the C-2v group, respectively. The authors' results are consistent with recent measurements of vertical electron attachment energies. (C) 2007 American Institute of Physics

Journal of Chemical Physics 126[19]. 2007.

P 129-07 "Electronic structure of xenon implanted with low energy in amorphous silicon"

Barbieri, P. F., Landers, R., de Oliveira, M. H., Alvarez, F., and Marques, F. C.

Electronic struture of Xe implanted in amorphous silicon (a-Si) films are investigated. Xe atoms were implanted with low energy by ion beam assisted deposition (IBAD) technique during growth of the a-Si films. The Xe implantation energy varied in the 0-300eV energy range. X-ray photoelectron spectroscopy (XPS), X-ray Auger excited spectroscopy (XAES) and X-ray absorption spectroscopy (XAS) were used for investigating the Xe electronic structure. The Xe M4N45N45 transitions were measured to extract the Auger parameter and to analyze the initial state and relaxation contributions. It was found that the binding energy variation is mainly due to initial state contribution. The relaxation energy variation also shows that the Xe trapped environment depends on the implantation energy. XAS measurements reveals that Xe atoms are dispersed in the a-Si matrix. (c) 2007 Elsevier B.V. All rights reserved

Journal of Electron Spectroscopy and Related Phenomena 156, 409-412. 2007.

P 130-07 "Energy spectra of exciton states in disk-shaped GaAs-Ga1-xAlxAs quantum dots under growth-direction magnetic fields"

Barticevic, Z., Pacheco, M., Duque, C. A., and Oliveira, L. E.

A theoretical study, within the effective-mass approximation, of the effects of applied magnetic fields on excitons in disk-shaped GaAs-Ga1-xAlxAs quantum dots is presented. Magnetic fields are applied in the growth direction of the semiconductor heterostructure. The parity of the excitonic envelope function related to the simultaneous exchange of z(e)->-z(e) and z(h)->-z(h) is a good quantum number and the wave function, both the odd and even parity, can be expanded as combination of products of the quantum well electron and hole function that preserves the parity with appropriate Gaussian functions. We have simultaneously obtained the energies of the excitonic ground and excited states and discuss the behavior of these energies as a function of the magnetic field

European Physical Journal B 56[4], 303-309. 2007.

P 131-07 "Entanglement in the dispersive interaction of trapped ions with a quantized field"

Semiao, F. L. and Furuya, K.

The mode-mode entanglement between trapped ions and cavity fields is investigated in the dispersive regime. We show how a simple initial preparation of Gaussian coherent states and a postselection may be used to generate motional nonlocal mesoscopic states involving ions in different traps. We also present a study of the entanglement induced by dynamical Stark shifts considering a cluster of N trapped ions. In this case, all entanglement is due to the dependence of the Stark shifts on the ions' state of motion manifested as a cross-Kerr interaction between each ion and the field

Physical Review A 75[4]. 2007.

P 132- 07"Exchange constant variation effects in magnetocaloric and barocaloric isothermal potentials"

Plaza, E. J. R. and Campoy, J. C. P.

Frequently, magnetothermal studies of many ferromagnetic materials are focused considering the system such as a paramagnet subject to a molecular field being characterized by an exchange constant. However, magnetostructural transitions can produce abrupt changes in the exchange constant triggering magnetic transitions of first order at transformation temperatures, which can be shifted by applying magnetic field or pressure. On thermodynamic bases we show how an abrupt but continuous variation of the exchange constant at the transition can play an important role in the magnetocaloric and barocaloric isothermal potentials in systems showing structural transformation

Physical Review B 75[17]. 2007.

P 133-07 "Exciton diamagnetic shifts in GaAs-Ga1-xAlxAs quantum dots and ultrathin quantum wells"

Barticevic, Z., Pacheco, M., Duque, C. A., and Oliveira, L. E.

A theoretical study of the growth-direction magnetic-field effects on the exciton photoluminescence peak energies in GaAs-Ga1-xAlxAs quantum-dot/ultrathin quantum-well systems is presented. Calculations are performed within the effective-mass approximation and taking into account nonparabolicity effects for both the conduction-band and valence-band effective masses. We use a simple 'QD + ultrathin QW' model heterostructure to mimic the actual physical system, and calculated results for the exciton diamagnetic shifts are found in overall agreement with recent experimental measurements.

Journal of Physics-Condensed Matter 19[21]. 2007.

P 134-07 "Experimental and theoretical spectroscopy of the aspirin in the UV/Vis region"

Mota, G. V. S., Pontes, A. N., Chaves, A. M. J., and Albuquerque, M. L. S

Journal of Electron Spectroscopy and Related Phenomena 156, LXI-LXI. 2007.

P 135- 07"Experimental and theoretical spectroscopy of the morphine in the UV region"

Mota, G. V. S., Pontes, A. N., Chaves, A. M. J., and Albuquerque, M. L. S.

Journal of Electron Spectroscopy and Related Phenomena 156, LXI-LXI. 2007.

P 136- 07"Experimental magnetic study and evidence of the exchange bias effect in unidimensional Co arrays produced by interference lithography"

Rosa, W. O., Knobel, M., Cescato, L., Gobbi, A. L., and Vazquez, M.

A simple process for fabricating submicrometric magnetic arrays employing interference lithography, sputtering deposition and lift-off processes is proposed and demonstrated. The magnetic properties of cobalt (Co) arrays were measured and compared with those of a continuous Co magnetic film. The results show a dependence of the hysteresis curve on the orientation of the field as regards the array, which is correlated with the anisotropy of the structures and a dependence of the coercive field on the periodicity of the arrays. Moreover, an exchange bias effect was observed, which is ascribed to a ferromagnetic/antiferromagnetic (FM/AFM) coupling between Co and a thin surface cobalt oxide (CoO) layer.

Solid State Communications 142[4], 228-231. 2007.

P 137- 07"Extended Grassmann and Clifford algebras"

da Rocha, R. and Vaz, J.

This paper is intended to investigate Grassmann and Clifford algebras over Peano spaces, introducing their respective associated extended algebras, and to explore these concepts also from the counterspace viewpoint. The presented formalism explains how the concept of chirality steins from the bracket, as defined by Rota et all [1]. The exterior (regressive) algebra is shown to share the exterior (progressive) algebra in the direct sum of chiral and achiral subspaces. The duality between scalars and volume elements, respectively under the progressive and the regressive products is shown to have chirality, in the case when the dimension n of the Peano space is even. In other words, the counterspace volume element is shown to be a scalar or a pseudoscalar, depending on the dimension of the vector space to be respectively odd or even. The de Rham cochain associated with the differential operator is constituted by a sequence of exterior algebra homogeneous subspaces subsequently chiral and achiral. Thus we prove that the exterior algebra over the space and the exterior algebra constructed on the counterspace are only pseudoduals each other, if we introduce chirality. The extended Clifford algebra is introduced in the light of the periodicity theorem of Clifford algebras context, wherein the Clifford and extended Clifford algebras Cl-p,Cl-q can be embedded in Cl-p+1,Cl-q+1, which is shown to be exactly the extended Clifford algebra. We present the essential character of the Rota's bracket, relating it to the formalism exposed by Conradt [25], introducing the regressive product and subsequently the counterspace. Clifford algebras are constructed over the counterspace, and the duality between progressive and regressive products is presented using the dual Hodge star operator. The differential and codifferential operators are also defined for the extended exterior algebras from the regressive product viewpoint, and it is shown they uniquely tumble right out progressive and regressive exterior products of 1-forms

Advances in Applied Clifford Algebras 16[2], 103-125. 2006.

P 138-07 "Field-emitter bound states in structured thermal reservoirs"

Mogilevtsev, D., Moreira, F., Cavalcanti, S. B., and Kilin, S.

We derive a master equation for a two-level emitter interacting with a band-gap reservoir at finite temperatures. This equation is able to capture effects of emitter-reservoir entanglement. We show that the entangled field-emitter bound state, which arises in the process of interaction, does not survive indefinitely at finite temperatures. However, such an entangled state may be effectively excited through an intensive incoherent driving

Physical Review A 75[4]. 2007.

P 139-07 "Glasses in the SbPO4-WO3 system"

Nalin, M., Poirier, G., Ribeiro, S. J. L., Messaddeq, Y., and Cescato, L.

Glasses in the binary system (100 - x)SbPO4-xWO3 (20 <= x <= 60, x in mol%) have been prepared and characterized. Differential thermal analysis (DTA) shows that the glass transition temperature, T-g increases from 412 degrees C, for samples containing 20 mol% of WO3 to 481 degrees C observed for glass containing 60 mol%. Sample containing 40 mol% in WO3 were observed to be the most stable against devitrification. The structural organization of the glasses has been studied by using Fourier transform infra-red (FTIR), Raman, P-31 Magic angle spinning (MAS) and spin echo nuclear magnetic resonance (NMR) spectroscopies. Results suggest two distinct networks comprising the glass structure, one with high SbPO4 content and the other characteristic of the highest WO3 content samples. The glasses present photochromic properties. Colour changes are observed for samples after exposure to ultraviolet or visible laser light. XANES, at L-1 absorption edge of tungsten, suggests partial reduction from W6+ to W5+ species during the laser irradiation. The photochromic effects and the colour changes, promoted by laser excitation, are reversible and easily removed by heat for during 1 h at 150 degrees C. Subsequent 'write/erase' cycles can be done without degradation of the glasses. (C) 2007 Elsevier B.V. All rights reserved

Journal of Non-Crystalline Solids 353[16-17], 1592-1597. 2007.

P 140-07 "High sensitivity absorption measurement setup for small metal clusters embedded in an argon matrix"

Conus, F., Tobias Lau, J., Rodrigues, V., and Felix, C.

Journal of Electron Spectroscopy and Related Phenomena 156, L-L. 2007.

P 141- 07 "Hydrogen storage in carbon nanoscrolls: An atomistic molecular dynamics study"

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

We report molecular dynamics results on the hydrogen uptake in carbon nanoscrolls (CNs), CNs are formed from helically wrapped graphite layers. We observed that at low temperatures significant H-2 storage is possible, but at higher temperatures thermal energies drastically reduce this capacity. Only a small fraction of hydrogen is adsorbed between scroll layers. Using temperature as the sorption/desorption variable we have observed that hydrogen can be released from the CN by temperature increase and can be readsorbed when the system is cooled. Higher capacities are expected if the CNs interlayer spacings are increased, making them an attractive nanostructure for H, storage having fast kinetics for charge/discharge. (C) 2007 Elsevier B.V. All rights reserved

Chemical Physics Letters 441[1-3], 78-82. 2007.

P 142-07 "Hydrostatic pressure and growth-direction magnetic field effects on the exciton states in coupled GaAs-(Ga, Al)As quantum wells"

Raigoza, N., Reyes-Gomez, E., Duque, C. A., and Oliveira, L. E.

The effects of hydrostatic pressure and growth-direction applied magnetic fields on the exciton dispersion and in-plane effective mass in coupled GaAs (Ga, Al) As quantum wells are investigated. Calculations for spatially direct and indirect excitons were performed within the variational procedure in the effective-mass and nondegenerate parabolic band approximations and by taking into account the coupling between the exciton centre-of-mass momentum and its internal structure. The pressure coefficient is also obtained as a function of both the hydrostatic pressure and growth-direction applied magnetic field

Journal of Physics-Condensed Matter 19[25]. 2007.

P 143-07 "Initial growth of Pd on Ru(0001): A multi-technique study"

de Siervo, A., De Biasi, E., Garcia, F., Landers, R., Martins, M. D., and Macedo, W. A. A.

Journal of Electron Spectroscopy and Related Phenomena 156, LXXXIII-LXXXIII. 2007.

P 144-07 "Investigating small fish schools: Selection of school - formation models by means of general linear models and numerical simulations"

Guimaraes, P. R., Bonaldo, R. M., Krajewski, J. P., Guimaraes, P., Pinheiro, A., Powers, J., and
dos Reis, S. F.

Journal of Theoretical Biology 245[4], 784-789. 2007.

P 145-07 "Investigation of the local Fe magnetic moments at the grain boundaries of the Ca2FeReO6 double perovskite"

Azimonte, C., Granado, E., Cezar, J. C., Gopalakrishnan, J., and Ramesha, K.

The local Fe ferromagnetic (FM) moment at the grain boundaries of a ceramic sample of Ca2FeReO6 double perovskite was investigated by means of x-ray magnetic circular dichroism spectroscopy at the Fe L-2,L-3 edges and compared to the overall bulk magnetization. We found that, at the grain boundaries, the Fe FM moments at H=5 T are much smaller than expected and that the MxH curve is harder than in the bulk magnetization. These results suggest a larger degree of Fe/Re antisite disorder at the grain boundaries of this sample, shedding light into the intriguing nonmetallic resistivity behavior despite the reported presence of free carriers. (c) 2007 American Institute of Physics

Journal of Applied Physics 101[9]. 2007.

P 146- 07"Magnetically frustrated behavior in multiferroics Mn2O5 (R = Bi, Eu, and Dy): A Raman scattering study"

Garcia-Flores, A. F., Granado, E., Martinho, H., Rettori, C., Golovenchits, E. I., Sanina, V. A., Oseroff, S. B., Park, S., and Cheong, S. W.

A temperature dependent Raman scattering study in multiferroic single crystals RMn2O5 (R=Bi, Eu, and Dy) was performed. The Raman spectra were measured in the range from 150 to 450 cm(-1) involving mostly Mn-O-Mn bending vibrations, complementing our previous work in a higher frequency range involving Mn-O stretching modes. A number of studied phonons present anomalous frequency behavior below a characteristic temperature, T*similar to 60-65 K, such as that found for the stretching modes. The sign and magnitude of such anomalous behavior appear to be correlated with the ionic radius of R, being softening for R=Bi and hardening for R=Eu and Dy in the range between T-C/T-N and T*. The anomalous phonon behaviors in both bending and stretching modes are consistent with an interpretation in terms of the spin-phonon coupling in a scenario of strong magnetic correlations. (c) 2007 American Institute of Physics

Journal of Applied Physics 101[9]. 2007.

P 147-07 "Magnetocaloric effect due to spin reorientation in the crystalline electrical field: Theory applied to DyAl2"

von Ranke, P. J., de Oliveira, N. A., Garcia, D. C., de Sousa, V. S. R., de Souza, V. A., Magnus, A., Carvalho, G., Gama, S., and Reis, M. S.

We report a way of obtaining the magnetocaloric effect due to the crystal electrical-field quenching of the total angular momentum in a magnetic system where a strong spin reorientation is present. The theoretical model is applied to DyAl2 and the results predict a considerable magnetic entropy change by rotating a single crystal in a fixed magnetic field. The obtained temperature and magnetic-field dependencies of the magnetization component along the < 111 >-crystallographic direction are in good agreement with the recently reported experimental data

Physical Review B 75[18]. 2007.

P 148-07 "Molecular dynamics simulation of single wall carbon nanotubes polymerization under compression"

Braga, S. F. and Galvao, D. S.

Single wall carbon nanotubes (SWCNTs) often aggregate into bundles of hundreds of weakly interacting tubes. Their cross-polymerization opens new possibilities for the creation of new super-hard materials. New mechanical and electronic properties are expected from these condensed structures, as well as novel potential applications. Previous theoretical results presented geometric modifications involving changes in the radial section of the compressed tubes as the explanation to the experimental measurements of structural changes during tube compression. We report here results from molecular dynamics simulations of the SWCNTs polymerization for small diameter arm chair tubes under compression. Hydrostatic and piston-type compression of SWCNTs have been simulated for different temperatures and rates of compression. Our results indicate that large diameter tubes (10, 10) are unlike to polymerize while small diameter ones (around 5 angstrom) polymerize even at room temperature. Other interesting results are the observation of the appearance of spontaneous scroll-like structures and also the so-called tubulane motifis, which were predicted in the literature more than a decade ago. (C) 2007 Wiley Periodicals, Inc

Journal of Computational Chemistry 28[10], 1724-1734. 2007.

P 149-07 "Monte Carlo simulations of hematite colloids"

Fonseca, P. T. and Castro, A. R. B. D.

Journal of Electron Spectroscopy and Related Phenomena 156, XCVI-XCVII. 2007.

P 150-07 "New constraints on ages of glasses proposed as reference materials for fission-track dating"

Laurenzi, M. A., Balestrieri, M. L., Bigazzi, G., Neto, J. C. H., Iunes, P. J., Norelli, P., Oddone, M.,Araya, A. M. O., and Viramonte, J. G.

New analyses have been performed in order to enhance the data-set on the independent ages of four glasses that have been proposed as reference materials for fission-track dating. The results are as follows. Moldavite - repeated Ar-40/Ar-39 age determinations on samples from deposits from Bohemia and Moravia yielded an average of 14.34 +/- 0.08 Ma. This datum agrees with other recent determinations and is significantly younger than the Ar-40/Ar-39 age of 15.21 +/- 0.15 Ma determined in the early 1980s. Macusanite (Peru) -four K-Ar ages ranging from 5.44 +/- 0.06 to 5.72 +/- 0.12 Ma have been published previously. New Ar-40/Ar-39 ages gave an average of 5.12 +/- 0.04 Ma. Plateau fission-track ages determined using the IRMM-540 certified glass and U and Th thin films for neutron fluence measurements agree better with these new Ar-40/Ar-39 ages than the previously published ages. Roccastrada glass (Italy) - a new Ar-40/Ar-39 age, 2.45 +/- 0.04 Ma, is consistent with previous determinations. The Quiron obsidian (Argentina) is a recently discovered glass that has been proposed as an additional reference material for its high spontaneous track density (around 100 000 cm(-2)). Defects that might produce "spurious" tracks are virtually absent. An independent Ar-40/Ar-39 age of 8.77 +/- 0.09 Ma was determined and is recommended for this glass. We believe that these materials, which will be distributed upon request to fission-track groups, will be very useful for testing system calibrations and experimental procedures

Geostandards and Geoanalytical Research 31[2], 105-124. 2007.

P 151-07 "Pd ultrathin film growth on C(0001): Does it show magnetic behavior?"

De Biasi, E., de Siervo, A., Garcia, F., Vicentin, F., Landers, R., and Knobel, M.

Ultrathin palladium metal films were grown on C(0 0 0 1). Their composition, electronic structure and magnetic behavior were studied by synchrotron based techniques (XPS and XAS), LEED and magnetic measurements. The Pd films were deposited in UHV conditions (pressure <5 x 10(-10) mbar) with thicknesses ranging from 1-2 to 12 ML. Annealing was performed to segregate Pd and to generate a cluster structure, which could induce the system to acquire magnetic properties as has been predicted by theoretical studies. To clarify the existence or not of ferromagnetic behavior in these samples, magnetic measurements were performed using a SQUID Magnetometer. (c) 2006 Elsevier B.V. All rights reserved

Journal of Electron Spectroscopy and Related Phenomena 156, 332-335. 2007.

P 152-07 "Photochromic properties of tungstate-based glasses"

Poirier, G., Nalin, M., Messaddeq, Y., and Ribeiro, S. J. L.

Vitreous samples were prepared in the NaPO3-BaF2WO3 ternary system with high WO3 concentrations. These glasses exhibit a strong absorption in the visible due to the presence of reduced tungsten species and the use of oxidizing species is required. The couple Sb2O3/NaNO3 was introduced in the composition and allowed to obtain transparent glasses. These oxidized samples were illuminated by visible laser radiation and showed an efficient volumetric photochromic effect. The photosensitive effect appeared as a dark spot throughout the entire volume of the glasses. The effect was investigated by several techniques such as, U-V-visible absorption, Raman and XANES at the L-1 and L-3 tungsten absorption edges. The results suggest a photoreduction of tungsten atoms without structural changes of the viteous network. Finally, the photochromic effect can be erased by thermal treatment at 200 degrees C for a few minutes. (C) 2007 Published by Elsevier B.V

Solid State Ionics 178[11-12], 871-875. 2007.

P 153-07 "Photoelectron diffraction study and structure determination of ultrathin hafnium silicide layers on Silicon(100) using MgK alpha radiation and synchrotron light"

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

Journal of Electron Spectroscopy and Related Phenomena 156, XXXV-XXXVI. 2007.

P 154-07 "Quantum conductance properties of atomic-size metal wires"

Ugarte, D.

Journal of Electron Spectroscopy and Related Phenomena 156, XXII-XXIII. 2007.

P 155-07 "Quantum state transfer between atoms located in coupled optical cavities"

Nohama, F. K. and Roversi, J. A.

We investigated the interaction between two coupled cavities, each one of them interacting with a two-level atom in its interior. We observed that if one of the atoms is in a superposition state and the other parts of the system are in their fundamental states, it is possible to transfer this state to the atom in the other cavity through the temporal evolution of the system. The time-evolution behaviour of the system during this transfer was studied and we observed its dependence with the frequency of the atom and the coupling constant between the atom and its respective cavity

Journal of Modern Optics 54[8], 1139-1149. 2007.

P 156-07 "Revising limits on neutrino-Majoron couplings"

Lessa, A. P. and Peres, O. L. G.

Any theory that has a global spontaneously broken symmetry will imply the existence of very light neutral bosons or massless bosons (sometimes called Majorons). For most of these models we have neutrino-Majoron couplings that appear as additional branching ratios in decays of mesons and leptons. Here we present an updated limit on the couplings between the electron, muon, and tau neutrinos and Majorons. For such we analyze the possible effects of Majoron emission in both meson and lepton decays. In the latter we also include an analysis of the muon decay spectrum. Our results are vertical bar g(e alpha)vertical bar(2)< 5.5x10(-6), vertical bar g(mu alpha)vertical bar(2)< 4.5x10(-5) and vertical bar g(tau alpha)vertical bar(2)< 5.5x10(-2) at 90% C. L., where alpha=e, mu, tau

Physical Review D 75[9]. 2007.

P 157-07 "Spatially indirect excitons in type-II quantum dots"

Madureira, J. R., de Godoy, M. P. F., Brasil, M. J. S. P., and Iikawa, F.

The authors have calculated the electronic structure for type-II InP/GaAs quantum dot systems considering a three-dimensional geometry including the wetting layer and the electron-hole interaction, which is the only responsible for the hole localization. Their results for the InP/GaAs structure show the electron confined inside the dot and the hole in the GaAs layer, partially above and below the dot. The authors propose structures with InGaAs or InGaP layers, where the hole wave function forms a ring around the dot walls. The electron-hole overlap, and therefore, the carrier lifetimes are very sensitive to the structural geometry, which is an important tool for device engineering. (c) 2007 American Institute of Physics

Applied Physics Letters 90[21]. 2007.

P 158-07 "Spectroscopy of rare gas clusters using VUV light from a free-electron laser"

de Castro, A. R. B., Bostedt, C., Eremina, E., Hoener, M., Thomas, H., Laarmann, T., Fennel, T., Meiwes-Broer, K. H., Plonjes, E., Kuhlmann, M., Wabnitz, H., and Moller, T.

Journal of Electron Spectroscopy and Related Phenomena 156, XXIV-XXIV. 2007.

P 159-07 "Structural and electronic properties of zigzag carbon nanotubes filled with small fullerenes"

Troche, K. S., Coluci, V. R., Rurali, R., and Galvao, D. S.

In this work we investigated the encapsulation of C-20 and C-30 fullerenes into semiconducting carbon nanotubes to study the possibility of bandgap engineering in such systems. Classical molecular dynamics simulations coupled to tight-binding calculations were used to determine the conformational and electronic properties of carbon nanotubes with an increasing fullerene concentration. We have observed that C-20 fullerenes behave similarly to a n-type dopant while C-30 can provide p-type doping in some cases. The combined incorporation of both types of fullerenes (hybrid encapsulation) into the same nanotube leads to a behaviour similar to that found in electronic pn-junctions. These aspects can be exploited in the design of nanoelectronic devices using semiconducting carbon nanotubes

Journal of Physics-Condensed Matter 19[23]. 2007.

P 160- 07"Structural and electronic analysis of Hf on Si(111) surface studied by XPS, XPD and ARXPS"

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

Journal of Electron Spectroscopy and Related Phenomena 156, XCIV-XCIV. 2007.

P 161-07 "Structural and electronic properties of atomic-size wires at low temperatures"

Lagos, M., Rodrigues, V., and Ugarte, D.

We have studied structural and electrical behavior of gold nanowires generated by mechanical elongation at liquid nitrogen temperature. Real-time observations using a low temperature sample holder in a high resolution transmission electron microscopy and, an ultra-high-vacuum compatible mechanically controllable break junction modified to cool the sample region have been used. It has been observed that the narrowest region of gold constrictions is crystalline and defect-free at room temperature, but this pattern is quite different at 150 K. Extended defects (e.g. twins) generate defective nanometer constrictions, indicating a very different structural evolution pattern during stretching. The generation of different atomic arrangements can be also deduced from transport measurements at low temperature. Finally, one-atom-size nanowires seem to be more stable at 150 K, as revealed by very long conductance plateaus at one quantum of conductance (lasting similar to 5-10 times longer than at room temperature). (C) 2007 Elsevier B.V. All rights reserved

Journal of Electron Spectroscopy and Related Phenomena 156, 20-24. 2007.

P 162-07 "Structural and electronic analysis of Hf on Si(111) surface studied by XPS, LEED and XPD"

Carazzolle, M. F., Schurmann, M., Fluechter, C. R., Weier, D., Berges, U., de Siervo, A., Landers, R., Kleiman, G. G., and Westphal, C.

In this work, we present a systematic electronic and structural study of the Hf-silicide formation upon annealing on Si(1 1 1) surface. The electronic structure and surface composition were determined by X-ray photoelectron spectroscopy (XPS) and angle-resolved X-ray photoelectron spectroscopy (ARXPS). To determine the atomic structure of the surface alloy we used low energy electron diffraction (LEED) and angle-resolved photoelectron diffraction (XPD). It was possible to verify that, after 600 degrees C annealing, there is alloy formation and after 700 degrees C the Hf diffusion process is predominant. Using LEED and XPD measurements we detected the ordered island formation simultaneously with alloy formation. (c) 2007 Elsevier B.V All rights reserved

Journal of Electron Spectroscopy and Related Phenomena 156, 393-397. 2007.

P 163-07 "Structural, chemical and electrochemical analyses of CuxV2O5 bronzes thin films"

Souza, E. A., Lourenco, A., and Gorenstein, A.

Vanadium pentoxide is one of the most attractive cathodic materials for use in microbatteries. However, the continuous insertion and extraction of lithium ions generate gradative losses in its intercalation capacity during the charge and discharge cycles. The insertion of metallic ions in the oxide matrix, forming bronzes of general formula MexV2O5 is an alternative to increase the electrochemical performance of V2O5. In this work, vanadium oxides and bronzes, in thin film form, were deposited by means of co-sputtering. Structural, chemical and electrochemical characterizations were realized in order to identify the cristallinity, composition, density and oxidation states of the elements in the film. The electrochemical techniques were used for analysis of the reversibility, charge capacity and determination of the diffusion coefficient for lithium ions. The main conclusion is that the addition of copper increased the specific volumetric capacity of the thin films and a better performance was attained during the charge/discharge cycles. (c) 2007 Elsevier B.V. All rights reserved

Solid State Ionics 178[5-6], 381-385. 2007.

P 164-07 "Study of the effect of neutrino oscillations on the supernova neutrino signal in the LVD detector"

Agafonova, N. Y., et al...

The LVD detector, located in the INFN Gran Sasso National Laboratory (Italy), studies supernova neutrinos through the interactions with protons and carbon nuclei in the liquid scintillator and interactions with the iron nuclei of the support structure. We investigate the effect of neutrino oscillations in the signal expected in the LVD detector. The MSW effect has been studied in detail for neutrinos travelling through the collapsing star and the Earth. We show that the expected number of events and their energy spectrum are sensitive to the oscillation parameters, in particular to the mass hierarchy and the value of theta(13), presently unknown. Finally we discuss the astrophysical uncertainties, showing their importance and comparing it with the effect of neutrino oscillations on the expected signal. We do not discuss in this paper the determination of oscillation parameters from the results of the observations; this task seems to be very difficult until astrophysical uncertainties are significantly reduced. (c) 2007 Elsevier B.V. All rights reserved

Astroparticle Physics 27[4], 254-270. 2007.

P 165-07 "Superconducting and magnetic behaviour of niobium doped RuSr2Gd1.5Ce0.5Cu2O10-delta"

Cardoso, C. A., Araujo-Moreira, F. M., Awana, V. P. S., Kishan, H., and de Lima, O. F.

Polycrystalline samples of Ru1-xNbxSr2Gd1.5Ce0.5Cu2O10-delta, 0 <= x <= 0.5, have been synthesized and structurally characterized by x- ray diffraction (XRD). Resistivity, magnetization and AC susceptibility measurements have been done and analysed considering a phase separation scenario. A strong suppression of the cluster glass (CG) transition associated with niobium doping was identified. In fact, the CG phase was not present in samples for x >= 0.2, leading to changes in the magnetic hysteresis loops measured at low temperatures. These hysteresis loops can be explained as a result of the contribution of two distinct magnetic phases: the canted AFM phase and embedded Ru4+- rich clusters which order as a CG in low temperatures. Interestingly, the significant changes in the magnetic response of the material do affect the superconducting transition temperature Tc. It was found that both Tc and the superconducting fraction are reduced in samples which present the spin glass phase. Therefore, our results point to some coupling between magnetism and superconductivity in this ruthenocuprate family, the presence of the magnetic moment being deleterious for the superconductivity

Journal of Physics-Condensed Matter 19[18]. 2007.

P 166-07 "Surface composition and structure of nickel ultrathin films deposited on Pd(111)"

Carazzolle, M. F., Maluf, S. S., de Siervo, A., Nascente, P. A. P., Landers, R., and Kleiman, G. G.

Journal of Electron Spectroscopy and Related Phenomena 156, XCVI-XCVI. 2007.

P 167-07 "Synthesis and characterization of NiO and NiFe2O4 nanoparticles obtained by a sucrose-based route"

Souza, E. A., Duque, J. G. S., Kubota, L., and Meneses, C. T.

Crystalline oxide powders were synthesized in nanoscale dimensions by a simple and novel chemical route, which is based on the use of sucrose as a chelating agent. The starting solutions were evaporated at 60 degrees C and the resulting gel was heated up to 300, 600 or 750 degrees C. The process was able to produce nickel oxide and nickel ferrite, characterized by structural and microscopic techniques. The average size of the particle was estimated by both Scherrer's equation and electron microscopy, and the results indicated that particles with a high crystallinity and a mean size in the range of 11-36nm were obtained. This synthesis route was able to produce NiFe2O4 and NiO nanoparticles at temperatures as low as 300 and 350 degrees C, respectively. (c) 2007 Elsevier Ltd. All rights reserved

Journal of Physics and Chemistry of Solids 68[4], 594-599. 2007.

P 168-07 "The construction of Dirac wave packets for a fermionic particle non minimally coupling with an external magnetic field"

Bernardini, A. E.

We shall proceed with the construction of normalizable Dirac wave packets for fermionic particles (neutrinos) with dynamics governed by a "modified" Dirac equation with a non-minimal coupling with an external magnetic field. We are not only interested on the analytic solutions of the "modified" Dirac wave equation but also on the construction of Dirac wave packets which can be used for describing the dynamics of some observable physical quantities which are relevant in the context of the quantum oscillation phenomena. To conclude, we discuss qualitatively the applicability of this formal construction in the treatment of chiral (and flavor) oscillations in the theoretical context of neutrino physics

International Journal of Theoretical Physics 46[6], 1562-1569. 2007.

P 169-07 "The coupling constants for an electroweak model with an SU(4)(PS) circle times SU(4)(EW) unification symmetry"

Bernardini, A. E.

We introduce the sequence of spontaneous symmetry breaking of a coupling between Pati-Salam and electroweak symmetries SU(4)(PS)circle times SU(4)(EW) in order to establish a mathematically consistent relation among the coupling constants at grand unification energy scale. With the values of baryon minus lepton quantum numbers of known quarks and leptons, by including right-handed neutrinos, we can find the mixing angle relations at different energy levels up to the electromagnetic U(1)(EM) scale

Communications in Theoretical Physics 47[5], 879-882. 2007.

P 170-07 "The effect of alloying on shake-up satellites: The case of Pd in SbPd2 and InPd2 surface alloys"

Pancotti, A., Carazzolle, M. F., Landers, R., de Siervo, A., and Kleiman, G. G.

Journal of Electron Spectroscopy and Related Phenomena 156, LXXIX-LXXIX. 2007.

P 171- 07 "The influence of the spin reorientation process on the magnetocaloric effect: Application to PrAl2"

von Ranke, P. J., de Oliveira, N. A., de Sousa, V. S. R., Garcia, D. C., de Oliveira, I. G., Carvalho,A. M. G., and Gama, S.

In this work we report a theoretical investigation about the influence of the spin reorientation on the magnetic and magnetocaloric properties of PrAl2. The model Hamiltonian takes into account the exchange magnetic interaction and the crystalline electrical field anisotropy. All theoretical results were obtained using the proper model parameters found in the literature for this compound. An anomalous valley was predicted to exist in the magnetocaloric curves for magnetic field changes along > 111 > non easy magnetic crystallographic direction. This anomaly was ascribed to the spin reorientation process. (C) 2007 Elsevier B.V. All rights reserved

Journal of Magnetism and Magnetic Materials 313[1], 176-181. 2007.

P 172-07 "Theory of microphase separation on side-chain liquid-crystalline polymers with flexible spacers"

Hernandez-Jimenez, M. and Westfahl, H.

We model a melt of monodisperse side-chain liquid-crystalline polymers as a melt of comb copolymers in which the side groups are rod-coil diblock copolymers. We consider both excluded-volume and Maier-Saupe interactions. The first acts among any pair of segments while the latter acts only between rods. Using a free-energy functional calculated from this microscopic model, we study the spinodal stability of the isotropic phase against density and orientational fluctuations. The phase diagram obtained in this way predicts nematic and smectic instabilities as well as the existence of microphases or phases with modulated wave vector but without nematic ordering. Such microphases are the result of the competition between the incompatibility among the blocks and the connectivity constraints imposed by the spacer and the backbone. Also the effects of the polymerization degree and structural conformation of the monomeric units on the phase behavior of the side-chain liquid-crystalline polymers are studied

European Physical Journal e 23[1], 31-42. 2007.

P 173-07 "Unconditional Bell-type state generation for spatially separate trapped ions"

Semiao, F. L., Missori, R. J., and Furuya, K.

We propose a scheme for the generation of maximally entangled states involving internal electronic degrees of freedom of two distant trapped ions, each of them located in a cavity. This is achieved by using a single flying atom to distribute entanglement. For certain specific interaction times, the proposed scheme leads to the non-probabilistic generation of a perfect Bell-type state. At the end of the protocol, the flying atom completely disentangles from the rest of the system, leaving both ions in a Bell-type state. Moreover, the scheme is insensitive to the cavity field state and cavity losses. We also address the situation in which dephasing and dissipation must be taken into account for the flying atom on its way from one cavity to the other, and discuss the applicability of the resulting noisy channel for performing quantum teleportation

Journal of Physics B-Atomic Molecular and Optical Physics 40[9], S221-S228. 2007.

P 174-07 "Use of CsCl to enhance the glass stability range of tellurite glasses for Er3+-Doped optical fiber drawing"

Rosa, C., Rodriguez, E. E., Chillcce, E. F., Osorio, S. P. A., Cesar, C. L., Barbosa, L. C., Mazali,I. O., and Alves, O. L.

Tellurite glasses are important as a host of Er3+ ions because of their good solubility and because they present broadband optical gain compared with Er3+-doped silica, with the potential to increase the bandwidth of communication systems. However, the small glass stability range (GSR) of tellurite glasses compromises the quality of the optical fibers. We show that the addition of CsCl to tellurite glasses can increase their GSR, making it easier to draw good-quality optical fibers. CsCl acts like a network modifier in glass systems, weakening the network by forming Te-Cl bonds. We show that the thermal expansion coefficient mismatch is in the right direction for optical fiber fabrication purposes and that the Bi2O3 content can be used to control the refractive index of clad and core glasses. Single-mode and multi-mode Er3+-doped optical fibers were produced by the rod-in-tube method using highly homogeneous TeO2-ZnO-Li2O-Bi2O3-CsCl glasses

Journal of the American Ceramic Society 90[6], 1822-1826. 2007.

Abstracta

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