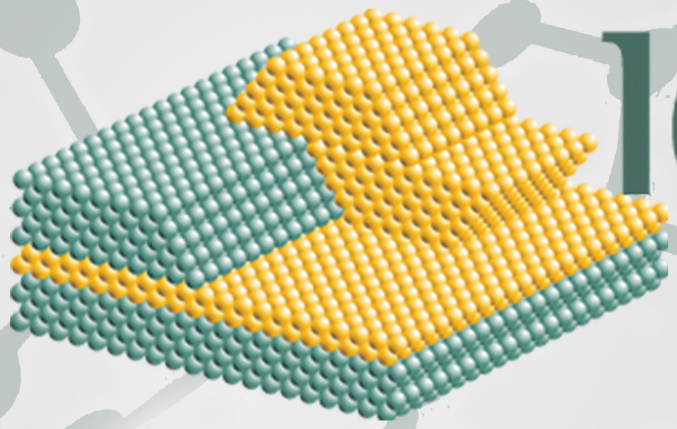

16th BWSP

Brazilian Workshop on Semiconductor Physics

Itirapina - SP - Brazil

May 05-10, 2013

ABSTRACT BOOK

CNPq Conselho Nacional de Desenvolvimento Científico e Tecnológico

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16th BWSP

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Abstract Book

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The Program

	sunday	monday	tuesday	wednesday	thursday	friday
8h30			Alegre	Teles	Amborsch-Draxl	Rahim
8h55		Parkin				Gordo
9h20			Felser	Van de Walle	Fuhrer	Micklitz
9h45		Malachias				
10h10			Dias de Moraes	S. O. Ferreira	Mendes	Zagonel
10h35		Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break
11h00		Gusev	Petta	Jungwirth	Molenkamp	Kudrawiec
11h25						
11h50		Hartmann	Samarth	Lee	Fabian	Deneke
12h15		dos Santos		Assali		Triffunovic
12h40		Cano	Dias da Silva	Viol Barbosa	Penello	
13h05		Almoço	Almoço	Almoço	Almoço	Almoço
13h30	Godoy (Tutorial)			excursion + adventure		
13h55						
14h20						
14h45	Egues (Tutorial)					
15h10						
15h35						
16h00	Coffee Break	G J. Ferreira	Freundlich		de Souza	
16h25	Fuhrer (Tutorial)	Ribeiro				
16h50		Leite Alves	Schoenhalz		Rino	
17h15	Zutic (Tutorial)	Koenraad	Pelá		Meet the Editors	
17h40		Coffee Break	Momtaz			
18h05		Oliveira	Cordeiro			
18h30	cocktail	Fernandes Lima	poster session 1		poster session 2	
18h55		Andrada e Silva				
19h20		Vernek				
19h45				dinner		
20h10					churrasco	

Summary

Talk Abstracts

Poster Abstracts

Abstracts of Talks

An Introduction to Dirac Electronic Materials

Michael S. Fuhrer[1]

[1]School of Physics, Monash University

The periodic potential imposed by the crystal lattice allows new effective Hamiltonians for electrons to be generated which may be qualitatively different than the Schrodinger equation for a free electron at low energies. I will discuss two striking recent examples. In graphene, the basis of two identical atoms in the honeycomb lattice leads to a massless Dirac Hamiltonian with an emergent spin-1/2 "pseudospin" spinor coupled to momentum. In the three-dimensional topological insulators, strong spin-orbit coupling leads to a Hamiltonian which is topologically distinct from the free-electron case, which gives rise to emergent metallic states at the boundaries (surfaces) of the material. These surface states also have a Dirac effective Hamiltonian, but with momentum coupled to the intrinsic electron spin. I will discuss how these materials are made, and how they are used to enable the study of Dirac electrons in the laboratory.

Application of electromodulation spectroscopy to study semiconductor structures containing quantum wells

Robert Kudrawiec[1]

[1]Institute of Physics, Wroclaw University of Technology

Electro-modulation spectroscopy [photoreflectance (PR) and contactless electroreflectance (CER)] is known as a very sensitive and nondestructive absorption-like technique to investigate the optical transitions in various semiconductor structures including transistor structures, quantum wells (QWs) and quantum dots [1-4]. Due to the Franz-Keldysh (FK) effect this technique can be also used to study the built-in electric field as well as the Fermi-level position at semiconductor surface, metal(dielectric)/semiconductor interfaces, or inside semiconductor structures [5, 6]. In this paper we are going to focus on various QW structures, which we recently investigated by using PR and CER. We are going to show the powerful of PR and CER spectroscopies in application to study the following issues. i) Energies of the ground and excited state transitions in QWs: Energies of QW transitions measured by PR (or CER) can be compared with theoretical calculations performed for various band gap alignment at QW interface. The energy level structure in the investigated QW (i.e., the number of confined electron and hole levels) can be determined comparing experimental data with these calculations. Here we show examples of application of PR and CER spectroscopy to study the band structure of GaInNAs/GaAs and GaInAsSb/GaSb QWs of various contents and widths. ii) Determination of energy gap for bulk-like layers in QW structures: QW structures for laser applications can contain a lot of bulk-like layers of different energy gap. Very often the energy gap of a given layer cannot be determined by photoluminescence measurements due to the carrier transfer to another layers e.g. QW region. The energy gap of QW barriers, step-like barriers and cladding layers can be measured by PR (or CER). The application of PR spectroscopy to study this issue will be presented within this point. iii) Built-in electric field: Here we are going to show the application of PR and CER to investigate the distribution of electric field in QW structures including the built-in electric field in p-i-n junction, the surface electric field and its influence on optical transitions in QWs located close the surface. iv) Homogeneity of QW structures: Broadening of PR and CER resonances related to QW transitions are very sensitive to QW inhomogeneities (i.e., fluctuation of QW width and QW content). Within this point we are going to show that QW inhomogeneities can be very well monitored by PR or CER in such material systems as GaInNAs(Sb)/GaAs and GaInN/GaN QWs. v) Carrier localization at low temperatures: Measuring the energy gap of fundamental transition in QW by PR (or CER) and comparing it with photoluminescence measurements it is possible to determine the energy of carrier localization in QW structures at low temperature as well as at higher temperatures. Examples of PR and CER studies of this issue for GaInNAs/GaAs and GaInN/GaN QWs will be presented within this point.

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Asymmetry tuning of the Fano lineshape in L3 photonic crystal cavities

Juan Pablo Vasco[1]; Pablo Thiago Valentim[1]; Herbert Vinck Posada[2]; Paulo Sergio Soares Guimaraes[1]

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Currently, semiconductor optics is focused on building high efficiency and low loss devices for optoelectronic applications. The control of the dissipation channels is fundamental for this purpose and thus constitutes an important and active research area. Semiconductor systems which present a spatially periodic dielectric function, known as photonic crystals, are optimal candidates for this purpose. Particularly, photonic crystal slab cavities show an interesting phenomena called Fano resonances, which are produced by the physical interference between quantized states of the cavity and the non-quantized, or external, continuum states through a dissipation channel, which is created by the finite thickness of the crystal. Therefore, changes of the lineshape of the Fano resonances changes the dissipation physical conditions. In this work we investigate the Fano resonances in two dimensional slab photonic crystal cavities of the type L3. These photonic crystals are fabricated on membranes of a semiconductor patterned with a periodic array of air holes. The actual cavity consists of three (L3) holes missing along one of the lines of the pattern. We calculate the Fano interference lines in the reflectivity through the scattering matrix method, with a defective periodic pattern described by a plane wave basis. We find that the Fano lineshape depends on the polarization of the incident field and the size of its circular shape. We show that for some polarizations angles the symmetry of the Fano resonance is reversed. The electric field inside and outside the structure is analyzed for a better understanding of the interference phenomenon. A comparison with experimental data on the reflectivity of photonic crystal cavities is also presented.

Atomic scale analysis of semiconductor nanostructures in 2 and 3 dimensions

Paul Koenraad[1]

[1]Department of Applied Physics, Eindhoven University of Technology

Present day semiconductor nano-science depends heavily on the construction of precise nanostructures in which atomic scale details are of key importance in the understanding and utilization of nanostructured semiconductor materials. It is thus essential to have microscopy techniques that allow such details to be assessed by techniques that can obtain true atomic resolution, preferable in 3 dimensions. Cross-sectional scanning tunneling microscopy and atom probe tomography are two techniques that are able to image semiconductor nanostructures at the atomic scale in respectively 2 or 3 dimensions. We will apply and compare both techniques on a range of interesting semiconductor nanostructures that were obtained by strain induced self-assembly or droplet epitaxy. We will show that both techniques are indeed able to obtain atomic scale information that is both unique and complementary, thus allowing unraveling details in the growth processes that remain elusive in many other analysis approaches.

Barium Sulfide: An Molecular Dynamics Simulation

José Pedro Rino[1]

[1]Universidade Federal de São Carlos

An effective two-body interatomic potential is proposed in order to study with molecular dynamics simulations the structural and dynamical properties of barium sulfide semiconductor. Barium sulfide, as other barium chalcogenides, are materials with technological interest due to its application as light emitting diodes, microelectronics, magneto-optics devices, and lasers diodes. The two-body interatomic potential proposed to describe BaS consider steric repulsions, Coulomb interactions due to charge transfer, charge-induced dipole attractions due to the electronic polarizabilities and van der Waals attractions are considered. With this effective pair-potential we are able to describe the vibrational density of states, heat capacity as a function of temperature, melting and its re-crystallization. The simulated results are compared with experimental observations and other calculations reported.

Catalyst influence on growth mechanisms and spontaneous diameter oscillations in Ag-catalyzed InP nanowires

Douglas Soares Oliveira[1]; Luiz Henrique Galvão Tizei[2]; Daniel Ugarte[1]; Monica Alonso Cotta[1]

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[2]Laboratoire de Physique des Solides, Université Paris-Sud, France

Semiconductor nanowires (NWs) are currently under intense investigation, both from a basic science point of view - to understand the dynamics of formation of these nanostructures – to a technological approach, due to their possible applications. However, these two lines of research share a common basis since the understanding of nanowire synthesis generally provide new features and applications. As an example, the catalyst material can dramatically change the morphology of the nanowire, but under the right growth conditions it can be used as a parameter for both growth control and modeling. We report here results on the growth of Ag-catalyzed InP nanowires, and discuss the precursor and temperature influence on the growth process. The microscopy analysis of the ensemble of our nanowires suggests that both vapor-liquid-solid (VLS) and vapor-solid mechanisms are present in our samples, giving rise to different nanowire morphologies and aspect ratios. We have proposed earlier that, for InP nanowire growth under high group III flows, there is a competition between different incorporation pathways of In atoms.This process may lead to a deformation on the triple-phase-line [Chiaramonte, T.; Tizei, L. H. G.; Ugarte, D.; Cotta, M. A. Nano Letters 2011, 11, 1934–1940],and eventually to mechanical instabilities of the nanoparticle position on top of the nanowire. Crystallographic phase changes may occur in this case, as well as sidewall wetting by the NP material. Under these conditions, spontaneous diameter oscillations form along InP nanowires grown with Au nanoparticles [Oliveira, D. S.; Tizei, L. H. G.; Ugarte, D.; Cotta, M. A. Nano letters 2013, 13, 9–13]. The mechanical stability of the nanoparticle on the top of the nanowire depends on the surface energiesinvolved in the problem. Thus changing the metal catalyst from Au to Ag, which has a lower surface energy, should alter the equilibrium conditions of the growth. Indeed, we observe different contact angles in this case. However, nanowire diameter oscillations are still present under different growth conditions than for the Au catalyst, suggesting these are general phenomena which occur under far from equilibrium conditions in VLS growth.

Cathodoluminescence mapping of localized light emission on III-V nanowire heterostructures

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[2]Laboratoire de Physique des Solides, Orsay, France

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Nanowires (NW) have opened a new way to form self-assembled heterostructures at the nanoscale. They also enable fabrication of nanowire-based devices with new functionalities by tailoring their band structure. Moreover, several studies have already used this approach and demonstrated single NW Light Emitting Devices (LEDs) and photodetectors. [1-4]. For studying optical properties of these nanostructures, full spectroscopic capabilities at high spatial resolution ($\sim$1 nm) become mandatory. Scanning transmission electron microscopes (STEM) equipped with high efficiency cathodoluminescence (CL) spectroscopy devices are now able to fulfil this requirement and image the sample structure at the same time. In this contribution, we will discuss recent results that correlate optical properties of III-V Quantum Discs (QDiscs) and other nanoscale insertions in NW with their morphology and structure. Sequences of three 15 nm thick InGaN inclusions within GaN nanowires have been analysed [3]. Due to the Volmer-Weber growth mode, these inclusions have an In gradient, as demonstrated by STEM-EDX, which possibly creates a band gap minimum on the top of the inclusion. In correlation to this morphology, CL maps show the emission to be most intense on the top on the InGaN inclusion. The increase of Indium on the inclusions is related to the elastic strain relaxation during growth. These findings elucidate the polychromaticity observed in InGaN insertions growth in identical conditions. GaN QDiscs with AlN barriers are subject to high carrier localization due to the high band gap difference between these materials. We have studied a sequence of 20 GaN/AlN QDiscs built within single NWs. Images show that the QDiscs thickness varies from 1 to 3.4 nm. Luminescence maps indicate clearly the energy difference between single QDiscs. QDiscs thicker than about 2.6 nm (10 monolayers) emit below the GaN band gap evidencing the Quantum Confined Stark Effect. Moreover, the growth of AlN on the side walls apparently creates a compressive strain that blue-shifts the emission of QDiscs of identical size. [2]. In this study, diffusion length of carriers is as short as about 5 nm.[5]

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Cavity enhanced light detection by resonant tunneling at telecommunication wavelengths

Fabian Hartmann[1]; Andreas Pfenning[1]; Fabian Langer[1]; Dirk Bisping[1]; Sven Höfling[1]; Martin Kamp[1]; Alfred Forchel[1]; Lukas Worschech[1]

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We have fabricated resonant tunneling diodes (RTD) based on GaAs/AlGaAs with a nearby and lattice-matched GaInNAs absorption layer for light detection at the telecommunication wavelengths. The electro-optical properties were investigated for different thicknesses of a thin GaAs buffer layer incorporated between the AlGaAs barrier and the GaInNAs absorption layer. RTD mesas with ring contacts and an aperture for optical excitation of charge carriers were fabricated with diameters from 12 μm down to 1 μm. A resonant current peak was observed for all samples at room temperature with a maximum peak-to-valley ratio of 3.9. Under illumination with laser light of 1.3 μm wavelength, a pronounced photo-effect is found. Further, the photodetector was embedded in an optical cavity consisting of alternating GaAs/AlAs distributed Bragg reflectors (DBR) with a resonance wavelength at $\lambda = 1.29$ μm. Photocurrent measurements showed sensitivities of 31 kA/W for resonant optical excitation and a quantum efficiency enhancement of 10 compared to off resonance excitation. The photodetector shows a resolution down to single photons.

Colossal Negative Magnetoresistance in Diluted Magnetic Semiconductors (GaMnAs)

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If you are in this job long enough to have witnessed the Berlin Wall for a little more than a decade, you can tell us about things like: the impossibility of having conduction in a two-dimensional system without an applied magnetic field; quantum Hall effect; Bohn-Aharanov effect in the gold ring; universal fluctuations of conductance; giant magneto resistance; and so on. These terms are all related with the surprising (at that time) effects of the magnetic field into "metallic" systems, most of them being high mobility semiconductor heterostructures. Aren't you satisfied yet? Well, then, now I can introduce you the colossal negative magnetoresistance, observed in mysterious alloys such as GaMnAs. And we have all the big stars ingredients: semiconductors, low dimensional systems, localization, many-particle effects, high temperature ferromagnetism, and so on. In this short lecture we will try to become acquainted with this interesting effect, after a survey of experimental results and a not so wide, let's call them so, collection of ansatz involving quantum interferences (like in the Bohn-Aharonov effect), spin-polarization and localization (a never found mobility edge resurges!), just to give you examples of some tentative theoretical explanations to the phenomena existing at present. Many more are certainly to come.

Combining the best of two worlds: organic/inorganic hybrid materials from first principles

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Hybrid materials composed by organic and inorganic components are most fascinating as new properties can arise at the interface, that are absent in either of the building blocks. Exciting examples thereof are organic molecules absorbed on graphene or encapsulated in carbon nanotubes, as being promising candidates for light-emitting devices [1,2]. I will discuss their properties covering structural conformation, electronic bands, and optical excitations as obtained from density-functional theory and many-body perturbation theory. It will be shown that though van der Waals interactions govern their bonding [3,4,5], the molecules and their inorganic counterparts interact in the excited state, giving rise to polarization-induced changes in electronic structure [5] and the formation of hybrid excitons [6].

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Complex oxides for next-generation electronics

Chris G. Van de Walle[1]

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The formation of a two-dimensional electron gas (2DEG) at the interface between two insulators, $SrTiO_3$ (STO) and $LaAlO_3$ (LAO), has sparked huge interest in oxide electronics. In spite of almost a decade of research, the mechanisms that determine the density of this 2DEG have not yet been unravelled. The polar discontinuity at the STO/LAO interface can in principle sustain an electron density of 3.3x10^{14} cm^{-2} (0.5 electrons per unit cell). However, experimentally observed densities are more than an order of magnitude lower.

We have used a combination of first-principles calculations and Schrödinger-Poisson simulations to investigate the origin of the electrons in the 2DEG at the STO/LAO interface. We have analyzed the nature of the heterostructures, in particular whether it is possible or not to form a second LAO/STO interface that does not act as a sink for electrons [1]. The inability to form a symmetric set of interfaces and the accompanying electric field in the LAO barrier layer ultimately limit the 2DEG density. The effects of different terminations of the LAO surface are examined.

Our results apply to oxide interfaces in general, and explain why the $SrTiO_3/GdTiO_3$(GTO) interface has been found to exhibit the full density of 0.5 electrons per unit cell [2]. We have also investigated the effects of strain on the band structure of STO [3], with the goal of guiding strain engineering to enhance the mobility in the 2DEG. Explicit first-principles calculations for both STO/LAO and STO/GTO heterostructures will be discussed.

Work performed in collaboration with L. Bjaalie, L. Gordon, and A. Janotti, and supported by the ARO and NSF.

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Conductance in a quantum wire: effect of equilibration

Tobias Micklitz[1]

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We study the effect of equilibration on linear and nonlinear conductances of spinless fermions in clean quantum wires. Equilibration of electrons in clean quantum wires is a very slow process since relevant scattering processes involve the band bottom. Large effects, therefore, only can be expected close to the conductance plateau transition where temperature is of the order of the band width. Close to the quantum phase transition where the conductance jumps from zero to one conductance quantum the conductance obtains an universal form governed by the ratios of temperature, bias voltage and gate voltage. Surprisingly, we find that for long wires the voltage predominantly drops close to one end of the quantum wire due to a thermoelectric effect [1].

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Density functional theory investigations of ZnO-organics interfaces

Aline L. Schoenhalz[1]; Gustavo M. Dalpian[1]; Thomas Frauenheim[2]; Andreia L. Da Rosa[2]

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In this work we investigate the structural and electronic properties of oxide semiconductor surfaces, ZnO in this case, functionalized with several organic molecules for different functionals. We have used the Density Functional Theory, and pay special attention in order to correctly describe the electronic properties of these systems. It is well known that the calculated energy band gap is almost five times smaller than the experimental one. Using local functionals such as LDA or GGA the energy gap is $\sim$0.8eV, whereas the experimental one is 3.4eV. This kind of problem can lead to wrong conclusions about the properties of the system and its application in optoelectronic devices (including sensors, dye-sensitized solar cells, ...), that have been designed by capping semiconductor surfaces with organic molecules, like the included by this study. Considering this, to develop this work we used a more accurate methodology, based on hybrid functionals (PBE0), to describe the exchange correlation term present in DFT. Besides the high computational cost, this functional provides a better description of the electronic properties of the studied material. We have studied the non polar (1010) ZnO surface, which is the dominant surface in ZnO nanowires. The adsorbed molecules, classified as anchoring groups, are the carboxilic acid (COOH), amine, thiol (SH), and glycine. Since GGA gives a reasonable description of the structural properties, we used the optimized structure with the GGA as the initial configuration for the PBE0 calculations. The analysis of the structural properties showed that there are no remarkable modifications in the structure when using the GGA or PBE0 functionals. Among the anchoring groups studied, both COOH and SH showed a dissociation of the molecules when adsorbed at the surface. From an electronic point of view, the changes are much more significant. For the PBE0, we observe a larger band gap, very similar to the experimental results (3.4eV for the hybrid functional). For the case of thiol, we observe more energy levels at the band gap with the hybrid functional than for the GGA. This occurs owing to the larger band gap of the PBE0. These results provide important insights into the nature of the interaction of organic molecules with the ZnO (1010) surface, showing that the use of hybrid functionals is mandatory in order to correctly describe this system.

Effects of disorder range and electronic energy on the perfect transmission in graphene nanoribbons

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[2]Universidade Federal Fluminense

[3]University of Central Florida

Numerical calculations based on the recursive Green's function method in the tight-binding approximation are performed to calculate the dimensionless conductance g in disordered graphene nanoribbons with Gaussian scatterers. The influence of the transition from short- to long-ranged disorder on g is studied as well as its effects on the formation of a perfectly conducting channel. We also investigate the dependence of electronic energy on the perfectly conducting channel. We propose and calculate a backscattering estimate in order to establish the connection between the perfectly conducting channel (with g=1) and the amount of intervalley scattering.

Phys. Rev. B 86, 205111 (2012)

Electronic and magnetic properties of rare-earth impurities in ZnO and GaN

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Wide bandgap semiconductors doped with rare earth (RE) impurities, received great attention over the last decade, mainly due to potential applications in optoelectronic [1] and spintronic [2,3] devices. Here, we perform a first principles investigation on the electronic properties of 4f-rare earth substitutional impurities (from Eu to Tm) in wurtzite gallium nitride and zinc oxide, using an all electron methodology plus an on-site Hubbard U correction (GGA+U). We show that a self-consistent procedure to compute that potential [4] provides an appropriate description of the 4f-related energy levels of RE ions. This is initially shown for the case of the metallic RE crystals, in which there are available experimental data [5] for comparison. We then use the same procedure to describe the RE as an impurity in GaN and ZnO, and compared with results from a recent phenomenological model [6,7], based on experimental data. The results indicate that the 4f-related energy levels remain outside the bandgap in both materials, in good agreement with that model. Additionally, zinc oxide doped with lanthanide impurities became an n-type material, independent of the Fermi level energy, showing a coupling between the 4f-related spin polarized states and the carriers, which may generate spin polarized currents, leading to applications in spintronic devices.

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Estimate of the photoinduced magnetic polaron radius in EuTe

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Europium chalcogenides (EuX) have the unique property of containing a very high magnetic moment (S=7/2) at every lattice site, associated with the half-filled 4f atomic orbital of the Europium atoms, and at the same time their energy bandgap is in the order of 2eV or larger, making them transparent at visible light. Therefore, if the spin order of the Eu atoms could be controlled at will using an external signal, this would make EuX an attractive material to be used as active component in magneto-optical and spintronic devices. In the case of EuTe, the natural ground state of the crystal lattice is an antiferromagnetoc arrangement. Recently, we demonstrated the induction of canted ferromagnetic in EuTe by using photons resonant with the bandgap of EuTe[1]. The canted ferromagnetic arrangement was achieved due to the generation photoexcited electrons in the lowest d-type conduction band. Once in the conduction band, the electrons have a strong d-f exchange interaction with the localized Eu spins, that favors ferromagnetic alignment of the lattice spins located within the reach of the electron's wave function, and competes with the f-f exchange, which favors antiferromagnetic arrangement, the end result being a canted ferromagnetic arrangement. The formation of the magnetic polaron becomes evident when it is observed that the external magnetic field required to reach full ferromagnetic arrangement decreases when photoexcited electrons are present. In this work we use ultra-low intensity photoluminescence measurements of the zero phonon emission (ZPL) as a function of temperature to investigate the magnetic polaron further. It is observed that when the temperature of the sample is scanned from below to above the Néel temperature, the ZPL first broadens up to the Néel temperature and then narrows again. The width of the ZPL is a signature of fluctuations of the spin arrangement within the radius of the photoexcited wave function, and is indeed expected to show a maximum at the Néel temperature. The temperature dependence of the ZPL width reflects the radius of the magnetic polaron. In order to obtain a quantitative estimate of this radius, Monte Carlo simulations were done. The input parameter in these simulations was the radius of the magnetic polaron, and it was varied in order to obtain the best fit of the temperature dependence of the ZPL width.

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Estructural characterization of CdMnTe/Si quantum dots

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Recently, great attention has been given to the development of new electronic devices for future information technologies based on manipulation of spins. Inserting magnetic ions in bulk II-VI semiconductors has been widely studied, leading to the first Diluted Magnetic Semiconductors (DMS) and, recently, the formation of quasi zero-dimensional magnetic polarons (i.e. regions with correlated carrier and magnetic ions spins) has been demonstrated in individual QDs. In this work we report the growth and structural characterization of CdMnTe quantum dots with very low Mn concentration, which are one of best system for this kind of studies. The samples investigated were grown by molecular beam epitaxy directly on Si(111) substrates, in contrast with the previously studied systems, where the DMS islands were grown on II-VI buffers layers. The use of Silicon as substrates is advantageous for its compatibility with most processes of the microelectronic industry. We have used atomic force microscopy, high resolution transmission electron microscopy and high resolution x-ray diffraction to investigate the effect of growth time and temperature on the morphology and structural characteristics of the quantum dots. Our results show that this system follows the Volmer-Weber growth mode and despite a lattice mismatch around 19%, highly perfect epitaxial islands can be grown. The introduction of Mn ions reduces the lattice mismatch and improves the structural quality of the islands, as observed by reciprocal space maps around the (111) Bragg reflection.

Hard X-ray Photospectroscopy: investigation of new materials

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Hard X-rays (3-10 keV) excite high-energy photoelectrons with a large inelastic mean free path, enhancing the probing depth of the photoemission technique. Hard X-ray photoelectron spectroscopy (HAXPES) has been proven to be bulk sensitive, and it allows the investigation of 3D systems since the contribution from surface effects (inhomogeneity, surface states) is strongly reduced in comparison to conventional XPS. This very versatile technique is especially suitable for multilayer and buried layer systems such as magnetic tunneling junctions (MTJ). In the same experiment one can selectively investigate interface properties, magnetic characteristics (magnetic circular dichroism in photoemission) and crystalline (x-ray photoelectron diffraction) ordering. The linear polarization dichroism can also be exploited to obtain symmetry information of bulk electronic states. We present some examples of HAXPES studies on Co and Mn-based Heusler films. Such class of Heusler material presents high spin polarization at Fermi energy and other promising features for the realization of spintronic devices. We investigate also other technologically relevant materials such as Bi_2Se_3 topological insulator and the VO_2 Mott transition systems using the HAXPES technique.

Heusler compounds: From semiconductors to spintronics

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Heusler compounds are a remarkable class of intermetallic materials with 1:1:1 (often called Half-Heusler) or 2:1:1 composition comprising more than 1500 members [1]. New properties and potential fields of applications emerge constantly; the prediction of topological insulators is the most recent example [2]. Surprisingly, the properties of many Heusler compounds can easily be predicted by the valence electron count or within a rigid band approach. The subgroup of more than 250 semiconductors is of high relevance for the development of novel materials for energy technologies. Their band gaps can readily be tuned from zero to 4 eV by changing the chemical composition. Thus, great interest has been attracted in the fields of thermoelectrics and topological insulator research. Ternary materials based on multifunctional properties, i.e. the combination of two or more functions such as superconductivity and topological edge states will revolutionize technological applications. The wide range of the multifunctional properties of Heusler compounds is reflected in extraordinary magneto-optical, magneto-electronic, and magneto-caloric properties. Tetragonal Heusler compounds Mn2YZ as potential materials for STT applications can be easily designed by positioning the Fermi energy at the van Hove singularity in one of the spin channels [3].

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HgTe as a Topological Insulator

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HgTe is a zincblende-type semiconductor with an inverted band structure. While the bulk material is a semimetal, lowering the crystalline symmetry opens up a gap, turning the compound into a topological insulator. The most straightforward way to do so is by growing a quantum well with (Hg,Cd)Te barriers. Such structures exhibit the quantum spin Hall effect, where a pair of spin polarized helical edge channels develops when the bulk of the material is insulating. Our transport data provide very direct evidence for the existence of this third quantum Hall effect, which now is seen as the prime manifestation of a 2-dimensional topological insulator. To turn the material into a 3-dimensional topological insulator, we utilize growth induced strain in relatively thick (ca. 100 nm) HgTe epitaxial layers. The high electronic quality of such layers allows a direct observation of the quantum Hall effect of the 2-dimensional topological surface states. Moreover, on contacting these structures with Nb electrodes, a supercurrent is induced in the surface states.

III-V dilute nitride aperiodic multi-quantum wells: a pathway for ultra efficient photovolatics

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The development of III-V multijunction devices incorporating 1 eV dilute nitride subcells has been often limited by poor minority carrier diffusion lengths encountered in bulk dilute nitrides. These short carrier diffusion lengths have led to severe degradations of device open circuit voltages and have to some extent impeded the development of efficient multi-junction photovoltaics. Previously we have shown that an alternate design, where dilute nitride quantum wells are inserted within the intrinsic region of a conventional GaAs p-i-n sub- cell could be used to overcome these limitations [1, 2]. Realization of such single junction device is shown to significantly improve the open circuit voltages compared to bulk-counterparts [3]. In addition negligible valence band offsets and the unusual increase of electron effective masses in dilute nitrides provide a unique opportunity to exploit aperiodic quantum well designs that through a resonant thermo-tunneling favor faster carrier escapes and near ideal carrier collection efficiencies [4]. The implementation of such designs is shown to provide a pathway toward the realization of ultra-efficient multi-junction devices with projected practical efficiencies approaching a staggering 50%.

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Indirect Interaction of Spins via Ferromagnet

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We propose a mechanism of long-range coherent coupling between spins coupled locally to a ferromagnet. An effective two-spin interaction Hamiltonian is derived and the coupling strength is estimated. We also discuss mechanisms of decoherence and consider possibilities for gate control of the interaction between neighboring spin-qubits. The resulting quantum computing architecture retains all the single qubit gates and measurement aspects of earlier approaches, but allows qubit spacing at distances of order 1 μm for two-qubit gates, achievable with the present-day semiconductor device technologies.

Kondo Correlations in Interacting Electron System

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Kondo effect is one of the most intriguing nonperturbative effects in condensed matter physics. Current theory of Kondo effect describes only noninteracting electrons occupying states directly interacting with a magnetic impurity (MI) while those electrons of the Fermi sea that do not interact with the MI are neglected. Recent fabrication of quantum dots (QDs) both doped with single magnetic Mn impurity and with controlled number of electrons opens the opportunity to investigate Kondo effect in interacting electron system.

In parabolic quantum dots doped with a single Mn ion in its centre only electrons that occupy zero angular momentum orbitals are directly coupled with Mn spin and those electrons in orbitals with finite angular momentum are not coupled with Mn spin. Therefore, these QDs are perfect candidates to investigate both the role of electron-electron interactions and the role of electrons in angular momentum channels that are not directly coupled with Mn on the Kondo physics.

We present here a microscopic model of N interacting electrons confined in a QD doped with a single Mn impurity. The Hamiltonian is composed of a kinetic energy, e-e Coulomb interactions, and electron-Mn exchange interaction (e-Mn). The e-Mn contact exchange interaction is described by a Heisenberg Hamiltonian. The QD electron single particle states are treated in the effective-mass approximation as states of a two-dimensional harmonic oscillator. The Hamiltonian matrix is constructed in the space of N electron configurations and M states of the MI. Using exact diagonalization techniques we calculate the eigenvalues and eigenvectors of our many-body Hamiltonian.

Here we show the results for a QD containing three and four electrons and Mn in the center of the QD. The ground-states of these two systems are built of electronic configurations with closed *s*-shell and a partially filled *p*-shell. Despite the fact that electrons in the *p*-shell do not interact with Mn spin, the spin of the electronic system is coupled with the spin of the Mn due to e-e interactions. The coupling is either ferromagnetic or antiferromagnetic depending of the number of empty confined shells in the QD. We show how this effective, e-e interaction mediated, coupling of *p*-shell electron spins with Mn spin can be detected in the photoluminescence spectrum. This work is supported by CAPES, FAPESP, NSERC and CIFAR.

Majorana fermions in topological quantum wires

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Majorana fermions in condensed matter systems have attracted a great deal of attention in the recent few years. They are zero-energy quasi particle excitations exhibiting the striking properties of being their own antiparticles. These quasi particles excitations have been predicted to appear in a variety of systems, such as quantum Hall setups, 2D topological $p_x + ip_y$ superconductors, topological p-wave superconductor quantum wires, etc. Despite of the theoretical progress on the predictions of such quasi particles, an experimental unambiguous detection is still lacking.

In this work we present a detailed study of Majorana fermions in a quantum wire coupled to metallic contacts within an extended version of the Kitaev model[1]. By performing an exact Green's function calculation, we show that the coupling to the leads introduces a broadening of the Majorana states bound to the ends of the wire. We also perform a careful investigation of the electron transport through a quantum dot coupled to one end of the superconductor quantum wire and to source and drain normal leads[2]. We find that for a long wire, as it is driven from its normal to its topological phase, the transmittance through the dot exhibits a smooth crossover from an expected single peak at $\hbar\omega = 0$ to a three-peak structure. For a very short wire, we find that the zero-energy value of the transmittance oscillates as the number of sites of the wire changes its parity. These oscillations vanish exponentially with the length of the wire.

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Micro and nanophotonics in optomechanical cavities

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Controlling the interaction between localized optical and mechanical excitations is now possible following advances in micro- and nano-fabrication techniques. In optomechanical crystals, the tight confinement, provided by the structure, to photons and phonons enhances the dynamical coupling between the optical and mechanical degrees of freedom. This optomechanical interaction can be used to modify both the phonon population and the refractive index of these systems. In this talk, we will discuss the basic principles of optomechanical interaction in cavities as well as new developments in this field. We will show how this nonlinear interaction can be used to create an all optical-tunable delay line. Finally, we discuss how we can efficiently cool down a mechanical mode to its quantum ground state, using optomechanical systems.

Microwave -induced magnetooscillatons in multilayer systems: Double and Triple quantum wells

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The observation of zero resistance is a rare phenomenon in condensed matter physics. Zero-resistance states (ZRS), which occur in two-dimensional electron (2D) systems exposed to a continuous microwave (MW) irradiation, are one remarkable example. Vanishing dissipative resistance appears at low magnetic fields induced by MW irradiation in samples with high quality (high mobility) [1]. This phenomenon has also attracted much theoretical attention [2]. Until now, all studies have been carried out in high- mobility 2D systems where one 2D subband is populated and experiments changing various parameters (such as MW frequency, power and temperature) have been reported. To date, there is no evidence for MW-induced ZRS in systems which are different from 2D with one occupied subband.

In this paper we give an overview of recent results on ZRS, microwave -induced resistance oscillations and MW-induced Hall resistance in bilayer and trilayer electron systems, which is regarded as MW-induced phenomena in 2DES.

We use high-mobility GaAs wide quantum wells (QW), double and triple QWs with different widths. In magneto-resistance, without microwaves, our system shows magneto-intersubband (MIS) oscillations thereby confirming the existence of two and three occupied subbands [3]. In bilayer systems a ZRS develops from the strongest minima of combined MIS-MIRO oscillations [3] which is different compared to single-layer systems [1]. This opens the opportunity for experimental and theoretical studies of ZRS in quasi-3D systems since we demonstrate that additional scattering (intersubband scattering [3]) is no hindrance for the observation of this intriguing phenomenon.

In addition we have studied the photoresponse of the Hall resistance R_{xy} in high-quality bilayer electron systems. Varying R_{xy} for different orientations of linear polarization strongly confirms the feasibility of polarization-dependent microscopic mechanisms of MW-induced Hall resistance, in contrast to polarization immunity in dissipative resistance.

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Mid-gap states and Kondo effect in disordered graphene

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Recent experiments on graphene flakes with short range scattering defects have renewed the interest on Kondo physics in graphene systems [1]. The experimental data show a temperature dependence of the resistivity consistent with the low-temperature Kondo screening of local magnetic moments.

Although recent theoretical explanations have been put forward [2,3], several questions remain open regarding the effect of short-range scattering and Kondo screening in such systems. It is important, for instance, to investigate how this would affect the local density of states in the vicinity of the impurities. In a localized state within a pristine graphene matrix, the linear dispersion in the density of states in graphene can lead to a pseudogap Kondo model [4] and a resulting rich variety of quantum critical behavior as a function of the gate-controlled chemical potential [5].

The presence of disorder changes this picture and favors the "standard" Kondo model, with a Fermi-liquid ground state coupled to an effective (disorder averaged) metallic band. Our goal is to study these effects with different numerical methods. Tight-binding calculations for diluted vacancies show the appearance of midgap states in the local density of states at the vicinity of the charge neutrality point, which is consistent with previous theoretical predictions [6]. The residual long-ranged disorder in the system couples these vacancy-induced localized states with the (disorder averaged) graphene DoS.

This motivates the formulation of an Anderson-like model with localized states within the graphene matrix, which may lead to Kondo screening consistent with the experiments. To investigate this possibility, we perform numerical renormalization group (NRG) calculations to study the Kondo temperature and transport properties for this model.

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Molecular beam growth of sub-monolayer and multilayer graphene on h-BN flakes

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We report the successful growth of graphene layers on h-BN substrate flakes in a MBE environment. The growth configuration was designed to allow a gradient in the deposition rate (DR) of carbon on the substrate. The growth conditions such as the substrate temperature were highly controlled. Characterization is carried out by spatially resolved Raman spectroscopy and by AFM imaging. We investigated the graphene coverage on the h-BN flakes. The flakes could be partially covered by a sub-monolayer film, fully covered by a single layer or fully covered by a multilayer film. We find high quality graphene in sub-monolayer and single layer growths. We found a striking independence on the carbon DR, which is attributed to the high mobility of carbons atoms on the h-BN surface. This is a characteristic feature of van der Waals molecular beam growth.

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Nonlinear transport and inverted magneto-intersubband oscillations in a triple quantum wells

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A two-dimensional (2D) electron system in a perpendicular magnetic field shows magnetoresistance oscillations, known as Shubnikov-de Haas oscillations (SdH) originating from the sequential passage of the Fermi level through Landau levels. If more than one subband is occupied the possibility of intersubband transitions start to occur and leads to another kind of magnetoresistance oscillation. These oscillations, called magneto-intersubband oscillations (MIS) have been studied in single quantum wells with two occupied subbands [1] and recently in a double quantum well (DQW) system [2] and triple quantum wells [3]. MIS oscillations offer new possibilities in transport measurements, e.g. the determination of quantum lifetimes in regions where SdH oscillations are completely suppressed at high temperatures [2, 3]. The nonlinear transport in two-dimensional 2D electron systems placed in a perpendicular magnetic field has been extensively studied in the past in connection with the Hall-field induced resistance oscillations (HIROs) [4] and zero differential resistance state phenomena [5]. Recently novel nonlinear effects in DQW have been observed: with increasing current I, the amplitudes of the MIS oscillations decrease, until a flip of the MIS oscillation picture occurs. In present paper we study the inverted MIS oscillations in TQW systems. Our samples are coupled GaAs triple quantum wells (TQWs) with a central well width of 20 nm and lateral well widths of 14 nm separated by a 1.4 nm barrier in a 2D electron gas with a mobility of 5×10^5 cm2 /Vs. The barrier widths are 1.4 nm and 2 nm, respectively. In our experiments, we have found that the current induced inversion of the magnetoresistance shows up in TQWs as a flip of the MIS oscillation pattern. We determine the critical magnetic field corresponding to the inversion of the quantum contribution to resistance for 3 different periods of MIS oscillations. Moreover, we compared the measurements for macroscopic size (500 μm) and mesoscopic size (5 μm) samples and found essential difference in the nonlinear transport behavior.

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Nonlocal transport near charge neutrality point in Two-dimensional topological insulator

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The two-dimensional(2D)topological insulator(QSHI)is characterized by a bulk energy gap and boundary modes that are robust to nonmagnetic impurities. The 2D quantum spin Hall insulator(QSHI)have been realized in HgCdTe quantum well with a width W ¿ 6.3nm. Indeed, the presence of the edge state transport in the absence of magnetic field has been recently demonstrated both in the ballistic [1] and diffusive cases [2] in HgTe quantum wells. This novel state is driven by the intrinsic spin-orbit interaction, which leads to the formation of the helical edge modes with opposite spins counter-propagating at a given edge. An unambiguous way to prove the presence of edge state transport in a 2DTI is the nonlocal electrical measurements. The application of the current between a pair of the probes creates a net current along the sample edge, and can be detected by another pair of the voltage probes away from the dissipative bulk current path. It has been shown that the resistance of HgTe quantum wells reveals a sharp peak, when the applied gate voltage induces an additional charge density, altering the quantum wells from an n-type to a p-type conductor via a QSHI state[1,2].The Hall Effect reverses its sign and Rxy =0, when Rxx approaches its maximum value, which can be identified as the charge neutrality point(CNP). These behaviors resemble the ambipolar field effect observed in Graphene [3]. The mechanism responsible for the observed peak of the local and nonlocal resistances near the CNP in HgTe quantum wells relies on the combination of the edge state and bulk transport contributions with the backscattering within one edge as well as bulk-edge coupling both taken into account. When the gate voltage is swept through the CNP the local and nonlocal transport coefficients arise from the edge state contribution at CNP and short-circuiting of the edge transport by bulk away from CNP. In this paper we provide details on the model taking into account the edge and bulk contribution to the total current. In the full edge + bulk transport model the density dependence of the local and nonlocal transport coefficients arises from bulk conductivity short circuiting the edge current away from the CNP. The model reproduces the key features of the data,in particular the density dependences of the local and nonlocal resistivity.

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Optical and magnetic properties of CeO2 films produced by combined spray pyrolysis

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With the emerging of the spintronics, the search for novel magnetic materials, with ideally large spin polarization and high TC, has become one of the main research lines in materials science. As a consequence, intense research on doping non-magnetic semiconducting oxides or insulating materials with magnetic ions has been developed. Ceria (CeO2) thin film is an interesting system to be studied because of its attractive physical properties such as large dielectric constant ($\sim$26) and wide band gap ($\sim$3.1 eV). In 2007, Fernandes et al. have shown that magnetic properties arise in pure ceria (which is essentially non-magnetic) as a result of the presence of oxygen vacancies [1]. In this work, we studied the optical properties of CeO2 thin films obtained by combined spray pyrolysis, using as precursor either cerium chloride or cerium acetate, deposited on Si(100) substrates. We performed Raman spectroscopy, Photoluminescence (PL), and Alternating Gradient-Force Magnetometry (AGFM) measurements in order to explore the connection between the defect bands and eventual magnetic properties of ceria films. We also performed X-ray Photoelectron Spectroscopy (XPS) for assessing the oxidation state of cerium in CeO2 films. Raman spectra showed the ceria line at 462-464 cm^{-1}, with narrow line width, indicating good quality films. PL results allow the separation of the samples into two categories: in the first the dominant structure is a defect-related recombination covering a wide range, from 1.9 to 2.4 eV, and in the second category the PL line shapes are dominated by a recombination around 3.1 eV. AGFM measurements, made on representative samples from both groups, showed a significant magnetic signal, directly correlated with the appearance of the defect bands in PL spectra. In order to investigate whether these magnetic signals are related to oxygen vacancies [1], XPS measurements were performed at Ce3+ and Ce4+ borders; these results agree with the AGFM and PL discussed above. This seems to allow us to suggest that a purely-optical, non-magnetic, simple experiment such as PL could be used to assess the existence of magnetic properties in ceria, and possibly in similar oxides. Raman measurements were performed at Raman Spectroscopy Laboratory, UFPR. We acknowledge financial support from CNPq, CAPES, and Fundação Araucária.

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Optical spin-transfer and spin-orbit torques

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Spin polarized carriers electrically injected into a magnet from an external polarizer can exert a spin transfer torque (STT) whose physical origin is a non-relativistic angular momentum transfer. The phenomenon belongs to the area of spintronics research focusing on the manipulation of magnetic moments by electric fields. A current induced spin-orbit torque (SOT) is a distinct relativistic phenomenon in which magnetization dynamics is induced in a uniform spin-orbit coupled ferromagnet in the absence of the external polarizer. In our femtosecond pump-and-probe magneto-optical studies of the ferromagnetic semiconductor (Ga,Mn)As [1], we observed an optical counterpart of the non-relativistic STT (OSTT) in which a circularly polarized pump laser pulse acts as the external polarizer [2]. We also report the observation of the optical counterpart of the relativistic SOT (OSOT) in (Ga,Mn)As [3]. The absence of an external polarizer in the OSOT corresponds to photo-carrier excitations by helicity independent pump laser pulses which do not impart angular momentum. The OSOT relies on spin-orbit coupling of non-equilibrium carriers, in a direct analogy to the current induced SOT.

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Photon-assisted Transport and Two-Stage-Kondo Effect in Quantum Dot Systems

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Electric transport in quantum dot systems is a subject of intense study nowadays, as they offer a unique opportunity for successful measurement of many-body-related phenomena.[1] For instance, Kondo physics, decoherence processes and entanglement are physical phenomena that can be investigate via transport measurements. It is in the fascinating area of spintronics[2] that quantum transport reveals its prolific potentiality in producing, for instance, spin polarized currents and quantum bits (qubits).[3] In the present work we apply a variety of techniques, like nonequilibrium Green function, master equation and numerical renormalization group to calculate conductance, current and magnetization of quantum dot devices. For a multi-impurity Anderson model we find that the two-stage-Kondo effect reported in previous works is drastically affected by the inter-dot Coulomb repulsion. In particular, we observe that the Kondo temperature for the second stage of the two-stage-Kondo effect increases exponentially with the inter-dot Coulomb repulsion, providing a possible path for its experimental observation.[4] we also investigate real-time dynamics of spin-polarized current in a quantum dot coupled to ferromagnetic leads in both parallel and antiparallel alignments. While an external bias voltage is taken constant in time, a gate terminal, capacitively coupled to the quantum dot, introduces a periodic modulation of the dot level. We find that spin polarized electrons can tunnel through the system via additional photon-assisted transmission channels. Owing to a Zeeman splitting of the dot level, it is possible to select a particular spin component to be photon-transferred from the left to the right terminal, with spin dependent current peaks arising at different gate frequencies. The ferromagnetic electrodes enhance or suppress the spin transport depending upon the leads magnetization alignment.[5] Finally, we analyze the spin polarized transport in a system composed of a ferromagnetic STM-tip coupled to an adsorbed atom on a metallic host surface. Electrons can tunnel directly from the tip into the surface or via the adatom. We analyze the interplay between both the lateral displacement of the tip and the intra adatom Coulomb interaction. Since the tip is ferromagnetic and the host metal is nonmagnetic we obtain a spin-diode effect when the adatom is in the regime of single occupancy. This effect turns into a polarized current for direct ($eV > 0$) and unpolarized current for reverse ($eV < 0$) bias voltage, if the tip is nearby the adatom.[6] This work was supported by the Brazilian agencies CNPq, CAPES, FAPESP and FAPEMIG.

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Property analysis of GaNAs alloy using GGA-1/2

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Current telecommunication techonology widely employs infra-red radiation in order to provide very fast fiber optic links, which enables quick and massive data transfer. To produce a semiconductor laser capable of emitting in such spectral region, the active medium should have a bandgap lower than the GaAs bandgap ($\sim$1.5 eV). Alloying between GaAs and GaN may provide a proper candidate for such task: although GaN bandgap is 3.5 eV, small addition of GaN to GaAs decreases GaAs bandgap dramatically, which allows an interesting bandgap engineering, from 1.5 eV to $\sim$0.5-0.8 eV (depending on growth conditions). However, the lattice mismatch between GaN and GaAs is very high ($\sim$20%), and it is expected a large miscibility gap considering typical growth temperatures (esides, for the first time, we constructed the phase diagram for this alloy, obtaining a critical temperature of $\sim$7000 K. These results provide an unique help for further experimental realizations of GaAsN.

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Putting Spin in Lasers

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Semiconductor lasers have been a fascinating research topic not only because of their versatile applications but also because of their rich physics as highly controllable nonlinear coherent optical devices. On the other hand, a number of efforts to understand spin phenomena in semiconductor have been continuously made and provided a breakthrough in information storage technology. However, the practical paths to room-temperature spin-controlled devices are typically limited to magnetoresistive effects. The interplay of spin injection into the lasers and their nonlinear coherent optical responses can lead to novel spintronic devices. Spin-polarized carriers in semiconductors can enhance the performance of lasers for large-capacity communication, signal processing and quantum cryptography [1]. While such spin-lasers already demonstrated a lower threshold current for the lasing operation [2] than their conventional (spin-unpolarized) counterparts in the steady-state, the most exciting opportunities come from their dynamical operation. We reveal that the spin modulation in lasers can lead to improvements in the two key figures of merit: enhanced bandwidth [3] and reduced parasitic frequency modulation—chirp [4]. The principles of spin modulation may also enable high-performance spin interconnects exceeding by orders of magnitude the information transfer available in conventional metallic interconnects [5].

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Quantum Interconnects for Spin Qubits

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A single electron spin in an external magnetic field forms a two-level system that can be used to create a spin qubit. Single spins are controlled using electron spin resonance and nearest neighbor spin couplings are achieved using the exchange interaction. A major challenge is to develop methods for coherently coupling spin qubits that are separated by large distances. I will describe our recent efforts to couple a spin qubit to a superconducting quantum bus in the circuit quantum electrodynamics architecture. Our results show that spin dynamics can be controlled using electric fields and the spin-orbit interaction[1,2,3]. We find that the microwave field of the superconducting resonator is sensitive to single spin dynamics. Our results suggest that a spin-cavity coupling rate of $\sim$1 MHz may be feasible, allowing spatially separated spin qubits to be coupled by a microwave field[4].

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Quantum well infrared photodetector based on GaAs/AlGaAs superlattice for CO2 detection

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It is proposed a system based on GaAs/AlGaAs heterostructure where the detection o CO2 is feasible. The structure is composed of a central quantum well (CQW) of GaAs which is embedded in a superlattice. The superlattice induces a minigap in the continuum (energies above the barriers) and the CQW acts as a defect, generating localized states inside the minigap. Adjusting the superlattice and the CQW thicknesses and the aluminum concentration, it is possible to tune the transition between the ground state to the continuum localized state occurs at the desired energy of 300 meV. The electronic states are calculated and it is verified the enhancement of the oscillator strength due to the transition from the ground state to the localized state in the continuum which is revealed in the high and sharp peak in the absorption spectrum. The dynamical response is obtained by solving the time-dependent Schrödinger equation using the split-operator method to calculate the photocurrent for several bias voltage and several radiation intensities. Besides the fact that the state is localized, the calculations confirm the generation of photocurrent when bias is applied as a result of the mixing of the localized state with extended states in the continuum. The calculated photocurrent spectra show an intense and acute peak around 300 meV and the energy position is weakly dependent on the bias.

Racetrack Memory: the current induced motion of domain walls by an interfacial chiral spin torque

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Electronic spin currents provide a powerful means of manipulating magnetization in magnetic memory and logic nano-devices. In particular, the transfer of spin angular momentum derived from currents spin-polarized by volume electron scattering gives rise to a spin transfer torque (STT) that can drive magnetic domain walls (DWs) along nanowires. This bulk-derived STT mechanism, however, weakens as the volume to surface ratio of the nanowire is reduced in ultra-thin magnetic layers: in this case the DWs are found to move in the opposite direction to that expected from bulk STT and, moreover, at much higher speeds1, 2. These properties are most pronounced in structures containing interfaces between atomically thin cobalt layers and platinum. Here we show that these properties are due to two intertwined phenomena both derived from spin-orbit interactions at the Co/Pt interfaces. By measuring the influence of magnetic field on current driven DW motion in perpendicularly magnetized Co/Ni/Co trilayers we find that there exists an internal effective magnetic field that operates on each DW. This field, localized at the DWs is oriented along the nanowire but has a direction that alternates between successive DWs, such that, acting in concert with spin Hall currents, the DWs are driven in lock-step along the nanowire. We propose that this chiral effective field arises from a Dzyaloshinskii-Moriya interaction (DMI) at the Co/Pt interfaces. By revealing the origin of this remarkable phenomenon that allows for the highly efficient manipulation of DWs in ultra-thin magnetic films, new families of spintronic devices can be anticipated, including Racetrack Memory, a high performance, and dense current controlled domain wall shift register3.

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Rashba models for quasi-one- and quasi-two-dimensional semiconductor heavy hole systems.

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One of the biggest challenges in Spintronics is the ability to efficiently manipulate spin currents in semiconductors systems without externals magnetic fields. Rashba spin-orbit interaction (SOI-R), is the more recurrent mechanism for achieving this, because its coupling parameter could be tuned *via* external electric fields. SOI-R for the heavy holes (hh) case is very different to the electrons or light holes (lh) case. Starting from a (8×8) Kohn-Lüttinger Hamiltonian and using the Quasi-Degenerate Perturbation Theory (Löwdin partition scheme), we obtain an effective SOI-R Hamiltonian, for a quasi-bidimensional hh system, with atypical cubic dependence on the wave number reported by Winkler *et al.*[**?**], and an expression for the coupling parameter which clarify the anomalous behavior[**?**] through the dependence on the difference of the hole levels energy. Comparisons with experimental data and previous models are shown. An effective SOI-R Hamiltonian for a quasi-onedimensional hh system is also obtained. Despite the lack of previous models to compare with, we find an expected linear term [**?**] as well as a cubic one. We include graphics of coupling parameters as a function of the hh density for different semiconductors in both cases.

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Recent Progress on LDA-1/2 method for gap correction

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For the past 30 years density functional theory (DFT) has been the dominant method for the quantum mechanical simulation of periodic systems, predicting the ground state properties of metals, semiconductors, and insulators with great success. This success not only encompasses standard bulk materials but also complex materials such as proteins, polymers, solids, nanostructures and DNA. Practical applications of DFT are based on approximations for the so-called exchange-correlation potential. Common approximations are the so-called Local Density Approximation (LDA) and Generalized Gradient Approximantion (GGA), which produce semiconductor band gaps significantly smaller than experiment. This fact raises the issue of how to obtain reliable excited-state properties. Recently, we addressed this question and propose a general form to calculate one-particle excitations in solids [1,2]. The method consists of calculating the self-energy as the quantum mechanical average of a "self-energy potential", which is added to the local part of the pseudopotential or to the -2Z/r part of the all-electron potential. We obtained band gaps of several semiconductors that compare very well with experiment, with the precision of the GW method, but at negligible computational cost. In this work we also present new developments of this method as the non self-consistent calculation for ionic compounds, as well as, its successful application to more complex systems as alloys, interfaces and magnetic semiconductors [3-5].

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Resistively Detected NMR and phonon-assisted dynamical nuclear polarization

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The resistively detected NMR (RDNMR) technique is used to detect the nuclear spin polarization and relaxation rates via magnetotransport in the quantum Hall regime. The diagonal term of the hyperfine coupling act on the electrons as an effective magnetic field Bn (Overhauser effect) proportional to the nuclear spin polarization. An oscillatory magnetic field with RF frequency in resonance with the nuclear spin splitting kills the nuclear spin polarization, and thus the effective magnetic Bn. This induces a change in the longitudinal resistance. Here we show that a finite current dynamically enhances the nuclear spin polarization via two processes: (i) near Landau level crossings a first order hyperfine spin-flip dominates, while (ii) away from crossings a second order phonon-assisted hyperfine spin-flip dominates. Our model show quantitative agreement with recent experiments [Zhang et al., PRL 98, 246802 (2007); Dean et. al., PRB, 80, 153301 (2009); Guo et al., PRB 81, 041306 (2010)]. See also [Ferreira et al., PRL 104, 066803 (2010)].

Spin effects in graphene structures

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The pz electrons of graphene carry no orbital momentum. Their spin-orbit coupling comes primarily from the hybridization with the dxz and dyz orbitals. The predicted splitting of the Dirac cones at K is about 25 micro eV. The same holds for derived structures such as bilayer And trilayer graphene, all the way up to graphite. If the inversion symmetry of graphene Is broken, new spin-orbit couplings appear. In an applied electric field transverse to graphene, for example, the Rashba spin-orbit fields cause spin splitting. But this splitting is rather small, on the scale of 10 micro eV for a rather strong field of 1 V/nm. Such values cannot explain the short spin relaxation time coming from spin injection experiments. Instead, it is likely that sp3 bonded adatoms produce giant local spin-orbit coupling by transferring the 10 meV spin-orbit coupling from the sigma to pi bands. The resulting local spin-orbit splitting is about 1 meV, two orders higher than in pristine samples. In addition, adatoms can induce local magnetic moments that also contribute to spin relaxation; first-principles calculations even predict that graphene with (nominally nonmagnetic) adatoms can become ferromagnetic. We demonstrate all these features on the example of recently experimentally investigated hydrogenated graphene, using first-principles and group-theory phenomenological calculations and discuss ramifications for spin-polarized transport.

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Spin injection in n-type GaAs/AlGaAs double barrier diodes

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We have studied the transport and optical properties of n-type GaAs/ AlGaAs resonant tunneling diodes (RTDs). Particularly, we have measured magneto-transport and polarized resolved photoluminescence of the devices as a function of applied bias voltage under magnetic field parallel to the tunnel current. By varying the applied bias, it is possible to change significantly the concentration of electrons and photo-generated holes tunneling through the device. As a consequence, the quantum well (QW) emission can comprise neutral, positively charged (X+), and negatively charged (X-) excitons, also known as trions. Two QW emission lines were observed for both right and left circularly polarized emissions under the electron resonant tunneling condition and attributed to the formation of neutral (X) and negatively charged excitons (X-) in the QW. The optical recombination between free holes (electrons) and confined electrons (holes) localized at the two dimensional electron gas, 2DEG (or two dimensional hole gas, 2DHG) formed at the accumulation layer next to the barriers (labeled 2DEG-h and 2DHG-e emissions) were also observed. The circular polarization degree from the QW emission for both lines is voltage controlled, with values up to -88% at 15 T at low voltages which are ascribed to an efficient spin injection from these 2DEG and 2DHG gases formed at the accumulation layers. The spin injection to the QW seems to be especially efficient under low voltages (before the electron resonance) when we observe a clear discrepancy between the relatively small spin-splitting energy and a rather large circular polarization degree. Under higher voltages, the QW polarization may depend on other additional effects, including the trion formation and the loss/gain of spin polarization during the tunneling processes into and out of the QW.

Spintronics; Basic Principles and Devices

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In modern information technology, charge-based logic is realized in semiconductor microprocessors, while ferromagnetic metals enable the use of carrier spin and associated magnetic moments for information storage. Advances in magnetic storage, recognized by the 2007 Nobel Prize in Physics, have enabled a 1,000-fold increase in the capacity of computer hard drives using metal-based spin-valves, over the last decade. This impressive success of spintronics applications has been typically realized in metal-based structures which utilize magnetoresistive effects for substantial improvements in the performance of magnetic sensors, computer hard drives, and magnetic random access memory (MRAM) [1-3]. However, this may only be the tip of the iceberg. A versatile control of spin and magnetism in a wide class of materials and their nanostructures, could also have a much broader impact leading to the new generation of multifunctional devices for spin logic and spin communication. Several basic principles [1-3] such as the generation, transport, manipulation, and detection of spin in solid-state systems, will be discussed. These principles will also help us to understand some surprising fundamental phenomena as well as to consider different emerging spintronics devices, including spin-based transistors[1,2], lasers [3], interconnects [4], and search engines [5].

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Strain engineering freestanding Si membranes by InAs overgrowth

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Freestanding membranes developed from single crystalline semiconductor structures have gained huge attention in the last years. Structures include stretchable electronics [1] as well as tunable InAs quantum dots transferred to a piezzo-electric substrate [2]. The structures rely on the detachment and transfer of high quality epitaxial defined heterostructures to a new host substrate. Recently it has been demonstrated, that partly release thin Si membranes emerging from Si-on-Insulator wafers are suitable templates for hetoroexpitaxial growth [3]. Hereby, the compliant substrate influences strongly the formation of self-assembled nanostructures (i.e. Ge islands on Si freestanding membranes).

The contribution reports on a work [4] using freestanding, compliant Si membranes with a thickness down to 10 nm as substrates for InAs self-assembled nanostructures. For the growth, freestanding Si membranes were defined and introduced into a MBE machine. In the subsequence, InAs was deposited and the growth monitored by reflective high energy electron diffraction. Furthermore, a systematic post-growth characterization by scanning electron microscopy, atomic force microscopy (AFM) and x-ray diffraction (XRD) was carried out. Our analysis shows that the thin Si membrane stays intact during the overgrowth and InAs island formation happens already after a sub-monolayer coverage of the sample surface. AFM shows a up bending of the freestanding membrane and indicates a different InAs island density on the freestanding, compliant parts compared to the ridged parts of the substrate. Finally, the strain analysis of the XRD data reveals a strain transfer of the islands to the compliant membrane. To further explain the results, finite element calculations were carried out indicating a non-uniform strain distribution of the islands from the inside of the membrane to the outside.

The results line out a new approach to strain engineer semiconductor materials and to integrate highly lattice miss-matched materials.

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Strain tailoring via novel semiconductor architectures: rolled-up tubes and nanomembranes

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The use of semiconductor thin films under pseudomorphic strain has been widely employed to modify structural, electronic and optical properties of epitaxial systems. Recently, novel approaches allow us to modify the strain initially introduced in thin films and embedded nanostructures during heteroepitaxy by methods such as MBE (Molecular Beam Epitaxy) or CVD (Chemical Vapor Deposition) [1]. In general terms, one or more strained films are deposited on top of a chemically sensitive layer, sitting on a single crystalline wafer. By selectively removing the chemically sensitive layer under well defined boundary conditions (lithographically defined) one can force the upper layers to roll-up into micro- and nanotubes or simply to detach from their original substrate [2, 3]. Such mechanisms can be therefore used to engineer the strain status of the released layers, inducing lattice configurations that cannot be achieved by any other method. In the case of detached nanomembranes, there is an additional possibility of transferring them to virtually any hosting substrate. In this talk we depict the modifications of strain in both kind of structures (tubes and membranes), using synchrotron x-ray diffraction [4, 5]. Applications of the resulting semiconductor architectures are also discussed [6, 7].

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Surface conduction of topological Dirac electrons in bulk insulating Bi_2Se_3

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The three dimensional strong topological insulator (STI) is a new phase of electronic matter which is distinct from ordinary insulators in that it supports on its surface a conducting two-dimensional surface state whose existence is guaranteed by topology. I will discuss experiments on the STI material Bi_2Se_3, which has a bulk bandgap of 300 meV, much greater than room temperature, and a single topological surface state with a massless Dirac dispersion. Field effect transistors consisting of thin (3-20 nm) Bi_2Se_3 are fabricated from mechanically exfoliated from single crystals, and electrochemical and/or chemical gating methods are used to move the Fermi energy into the bulk bandgap, revealing the ambipolar gapless nature of transport in the Bi_2Se_3 surface states. The minimum conductivity of the topological surface state is understood within the self-consistent theory of Dirac electrons in the presence of charged impurities[1]. The intrinsic finite-temperature resistivity of the topological surface state due to electron-acoustic phonon scattering is measured to be 60 times larger than that of graphene largely due to the smaller Fermi and sound velocities in Bi_2Se_3[2], which will have implications for topological electronic devices operating at room temperature. As devices are made thinner, we observe a crossover in weak anti-localization behavior from two decoupled topological surfaces (top and bottom) to a single coupled coherent topological system[3]. In the thinnest Bi_2Se_3 samples ($\sim$3 nm) we observe the opening of a bandgap due to coupling of the top and bottom surfaces which hybridize to form a conventional two-dimensional insulator[4], and by controllably thinning regions of Bi_2Se_3 samples we achieve quantum dots with gate-tunable insulating barriers[5].

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The interesting optical range of semiconductors

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Talking about semiconductor physics between experts always help us to clarify the ideas and solutions about our specific problems, such as the development of a new product or our undergraduate/graduate work. However we can lose the general overview of applications which allow us to motivate the search for new challenges or just the introduction of your doctorate thesis. Since the semiconductors present an optical characteristic due to their bandgap nature, we present a short review of spectroscopy properties and existing devices in specified spectral regions, the popular materials and the used structures as well as some important characteristics which can be mapped by photoluminescence spectroscopy in an introductory approach.

Theoretical investigation of the pressure-induced structural phase transitions of XTe (X = Ge, Sn, Pb) compounds

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Nowadays, thermoelectric (TE) materials that convert heat flux directly into electrical power have enormous promise in dealing with the challenges of the growing demand for alternative clean energy, and are a subject of great scientific interest. Te-based materials (i.e., PbTe, SnTe, and GeTe) are well-known candidates for medium-temperature TE devices. However, while PbTe has been object of investigation already for several years, little is known about both GeTe and SnTe: SnTe, at standard conditions, crystallizes in the NaCl structure (B1, stable up to 1000 K), while GeTe is found at face centered rhombohedral modification, with Ge and Te atoms being displaced from ideal rocksalt sites. Solid-state studies have shown a low temperature cubic α-SnTe to rhombohedral β-SnTe phase transition which occurs around 100 K and, for GeTe, it was shown that a phase transition to the rocksalt structure occurs at 670 K. On the other side, at intermediate pressures (≈ 6 GPa), PbTe transform from the B1 modification to an orthorhombic crystalline phase that was only recently experimentally confirmed to be of Pnma symmetry. At pressures of ≈ 25 GPa, it undergoes the CsCl structural phase (B2). In the present work, we report on the results of ab initio calculations of the Vinet equation of state, thermodynamic properties and both the pressure- and phonon-induced structural phase transitions of PbTe, SnTe and GeTe. The calculations were carried out by using the Density Functional Theory within the Local Density Approximation, gradient conjugated techniques, and the plane-wave pseudopotential method (*Abinit* code). We have used the Troullier-Martins pseudopotentials, and the thermodynamic related properties, were obtained by means of the anharmonic approximation (*Gibbs* code). Our results are in very good agreement with both the available experimental data and other theoretical calculations, whenever these comparisons are possible. From the obtained results, we show that these materials have soft acoustic modes which are responsible for the observed low-pressure phase transitions, giving the corrected pressures for the observed phase transitions.

Topological Insulator Heterostructures: Searching for Exotic Particles on a Bench Top

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Recent theories of "topological insulators" [1,2] have shown that in the complex and emergent world of condensed matter physics, one can engineer the interplay between fundamental symmetries, band structure and spin-orbit coupling to create novel energy-spin-momentum relationships for band electrons and to yield the effective realization of exotic particles predicted but yet unobserved in Nature. This talk will describe the experimental routes we are pursuing to build "detectors" for such particles, by coupling the surface states of a topological insulator with the gauge symmetry breaking effects of superconductivity [3] and the time-reversal symmetry breaking effect of ferromagnetism [4-6].

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Tunable phase in the spin coherence generation of self-assembled (In,Ga)As quantum dots

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In the last decades semiconductor physics has experienced a revolution in regard to manipulating electron spin, which lead to the birth of a new technology – spintronics. The spin of an electron resident in a quantum dot offers an opportunity to store spin information over much longer time scales than in two- or three-dimensional quantum structures. In this work the focus our attention in an ensemble of self-assembled (In,Ga)As quantum dots embedded in a GaAs host crystal. The GaAs was modulation doped with Si, such that each quantum dot contains one electron on average. The electron spin vector in a given quantum dot of the unperturbed ensemble can point in any direction with equal probability, therefore the net spin magnetization is zero. However, by illuminating the ensemble with circularly polarized light resonant with the fundamental energy gap of the quantum dot, the spin in individual dots can be made to become oriented along the light's wave vector, thus spin coherence is generated in the ensemble. In this work we investigated spin coherence generation using circularly polarized pump pulses of picosecond duration. The magnetization induced by the pump pulses was deduced by measuring the Faraday rotation of a linearly polarized probe pulse. Using an optical delay line, the time interval between the pump and probe pulses could be adjusted, thus time-resolved spin coherence could be investigated with femtosecond precision. By applying a variable magnetic field perpendicular to the light wave vector (Voigt geometry), the light-induced magnetization of the quantum dot ensemble was made to precess around the direction of the magnetic field. The frequency of the Faraday rotation signal measures directly the gyromagnetic factor of the electrons resident in the quantum dots [1]. Here we concentrate on the phase of the Faraday rotation signal. We show that it is dependent on the exact value of the excitation photon energy, on the pump pulse area (i.e. integrated pump pulse intensity) and on the intensity of the applied magnetic field. The phase dependence on external parameters is associated with the quantum dot energy level structure, which determines the microscopic mechanism of spin coherence generation.

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Twisted spins

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In this tutorial I will review the basics of the spin orbit interaction in semiconductor heterostructures. By following a "folding down" procedure akin to the Löwdin perturbation theory or the Schrieffer-Wolff transformation, I will derive effective Hamiltonians for electrons. As a first example I should show how to obtain the Pauli equation (plus spin orbit) from the Dirac equation. Then I will derive the so-called Rashba spin orbit interaction in structurally symmetric and asymmetric quantum wells. The Rashba interaction underlies many interesting physical phenomena in two-dimensional electron gases, e.g., the robust spin density wave pattern termed Persistent Spin Helix (PSH) and the relativistic Zitterbewegung, both to be briefly discussed as well. Finally, I will also touch upon recent developments and the renewed interest in spin orbit coupled systems such as quantum wires and wells and cold atomic gases as convenient platforms to investigate and probe topological insulators and Majorana fermions.
Research at IFSC/USP on the above topics is funded by CAPES, CNPq, FAPESP and the Research Support Center initiative of the PRP/USP (NAP Q-NANO).

Abstracts of Posters

8×8 Kane model for the electronic structure of wurtzites

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The spin-orbit interaction has played a crucial role in the development of low-dimensional semiconductor devices. In recent results addressing the 8×8 Kane model for cubic systems, particularly zincblende lattices, effective hamiltonians for the conduction band are calculated in a semi-analytical way. By folding down the Kane hamiltonian, the spinor components in the conduction band are isolated, resulting in an equation having the energy in denominators. Through a linearization process, controlled by a power expansion in the inverse of the energy gap, the energy is removed from the denominators and an effective hamiltonian is obtained. In a zincblende system, terms dependent on spin only appear in the effective hamiltonian of second order in the inverse of the energy gap of a heterostructure [PRL 99, 076603 (2007); PRB 78, 155313 (2008)]. In this work we apply this semi-analytical procedure to generate effective hamiltonians for the conduction band of wurtzite systems. Using the symmetries of the hexagonal lattice, the 8×8 Kane model is reviewed by taking into account all couplings mediated by the linear momentum and spin angular momentum. We show that exists an unified treatment for the Kane model of zincblende and wurtzite systems, which can be very useful in studies with nanowhiskers. We have found a first-order effective hamiltonian having terms dependent on spin even in the bulk case. One of these spin-dependent terms is the helicity operator. The spin-orbit interaction only appears in the second order expansion. Considering the first order hamiltonian, we have calculated the *Zitterbewegung* effect and discussed the Datta-Das transistor. We have found that only the spin operators exhibit the *Zitterbewegung* effect. The linear dependence with time shown by the position operators make of the spin operators harmonic fields, which form spin grattings similar to those found in zincblende heterostructures (persistent spin helix). We have also included a radiation field and calculated the (direct) optical transitions assisted by spin. We have found that the transition rates are harmonic functions of the incidence angle.

A comparative investigation of the redox potential in LiFePO4 and LiMnPO4 olives.

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The improvement of the performance and production cost of energy storage devices such as Li-ion batteries are considered, nowadays, key points to finally substitute a pollutant energetic matrix to an environmental friendly and sustainable energetic matrix [1]. Thus, the understanding of properties such as the open circuit voltage and the electronic structure become important to improve even more its performance and cost of production in these devices. The main idea of this work is to compare the accuracy of conventional semi-local density functional theory DFT for redox reaction energies with the Tran-Blaha modified Becke-Johnson semi-local density approximation [2, 3]. This is a parameter free method in which the exchange term is treated by the modified Becke-Johnson (MBJ) potential and the correlation term is treated within the local or semi-local density approximation. The electronic structure properties of LiFePO4 and LiMnPO4 together with their delithiated states (FePO4 and MnPO4) are investigated. A comparison between the predicted open circuit voltage in these materials is showed considering the Generalized Gradient Approximation and the MBJ method.

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A study of the magneto-transport near the charge neutrality point in the Quantum Hall Effect regime in graphene

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In this work we propose the study of the transport properties in single layer and bilayer graphene at the charge neutrality point (CNP) and compare it with random magnetic model developed in theoretical papers [8,9,10]. We argue that at CNP graphene layer is still inhomogeneous, very likely, due to random potential of impurities. The random potential fluctuations induces smooth fluctuations of the local filling factor around v=0. In this case the transport is determined by special class of trajectories, "the snake states" [8] propagating along contour v=0. The situation is very similar to the transport of a two-dimensional particles moving in a spatially modulated random magnetic field with zero mean [9]. We specially emphasis that our results may be equally relevant to the composite fermions description of the half-filled Landau level [10]. In addition we propose the study of the graphene resistance in the tilted magnetic field. It is expected that the graphene sheet is not a planar and some kind of static ripples deform the layer shape. Since the two dimensional electron gases is sensitive to only the normal component of the magnetic field B, electrons confined to a no planar layer experience nonuniform magnetic field varying with position depending on the surface shape, if an uniform B is applied to such nonplanar surface.

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10. Composite Fermions: A Unified View of the Quantum Hall Regime by O. Heinonen

Adiabatic Electron Pumping through Graphene-based Nanoelectromechanical Resonators

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We theoretically investigate the adiabatic electronic transport through graphene-based nanoelectromechanical resonators. The device is modeled by an effective long-wavelength Hamiltonian (given by the Dirac equation) for the electrons and using the continuum elastic theory for the mechanical motion. One obtains the equations of motion describing the system dynamics employing a non-equilibrium Green's function theory. Due to the mutual coupling between the electronic and mechanical degrees of freedom, both sets of equations have to be solved self-consistently. We present analytical and numerical results of the pumped charge and the mechanical response for a typical resonator setup. We also discuss the role of non-adiabatic corrections and the resulting damping of the mechanical motion.

An Extended Hückel Study of the Band Gap of III-V Alloys

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III-V alloys are systems widely studied both experimentally and theoretically, and some of these alloys display direct-indirect band gap crossover when the concentration x of the group V element is varied. On the other hand, standard density functional theory (DFT) calculations based in both LDA and GGA approximation are unable to reproduce the correct value of the concentration x_c for the band gap crossover. In this study, we present tight-binding (TB) calculations of the dependency of the band gap energy on the concentration of two ternary alloys: $GaAs_{1-x}P_x$ and $Al_xGa_{1-x}As$. Both systems demand the use of large supercells in order to get a significant description of the alloys, leading to high computer demands despite the recent development of highly efficient *ab-initio* DFT-based formalisms that scale linearly with the number of atoms. As an alternative procedure, it is common to approach the problem using semi-empirical tight-binding hamiltonians that employ linear combination of atomic orbitals (LCAO) for basis sets, with orbital energies and hopping parameters fitted to accurate band-structures as described in the seminal paper of Slater and Koster. One such example is the semi-empirical Extended Hückel Theory (EHT) method for electronic calculations for periodic and non-periodic systems, employed due to its simplicity and the chemical insight it provides. The EHT presents the following advantages over the traditional orthogonal TB schemes: (*i*) a considerable reduction in the number of parameters to be adjusted; (*ii*) natural scaling laws for the atomic orbitals' interaction and, (*iii*) an enhancement of the transferability of the parameters for different chemical environments. In this work, we perform EHT calculations for obtaining the alloy spectra, using a spd as valence basis set for each atomic species. For each atom type, atomic orbitals are expanded in terms of two Slater-type orbitals (double zeta basis set), where the parameters relative to each Slater orbital and the expansion coefficients were generated using a simulated annealing approach. We find that our results for the crossover concentrations are in better agreement with experimental than the ones obtained DFT calculations.

Analysis of properties and fabrication process of Infrared quantum well photodetectors.

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Computational models to aid the design of Quantum Well Infrared Photodetectors, QWIPs, have been focus of several papers since the eighties. Several numerical methods are applied to compute eigenenergies and eigenfunctions, to estimate the intensity of dark current and photocurrent, absorbance spectrum, and so on. A set of these tools are useful in order to master the development of QWIPs. The development of nanostructured infrared sensors based on quantum wells (QWIPs) and quantum dots (QDIPs) have received considerable attention of some research institutions and Universities in Brazil. We have been developing several numerical methods to aid the design of QWIPs which have been tested by comparing our results with the ones presented in the literature. As an important step to master the entire fabrication process in Brazil, these methods have been recently used to design sensors to detect radiation with wavelengths around 4.3 and 9.5 micrometers. Such sensors were fabricated and some important parameters, dependent of material and fabrication process, have been determined. In this work we present an analysis, by using some of these numerical approaches, of two samples of QWIPs cut from the same wafer grown by MBE, and processed using different infrastructures and operators. The heterostructure was designed by using a software program based on the finite element method and computational optimization techniques. The QWIP's were compound by AlGaAs (barrier layers) and GaAs (well layers) with detection wavelength peak in 9.3 μm. Dark current measures, of both samples, were performed at different temperatures with the samples located together at the same equipment. For temperatures higher than 60K, a difference around an order of magnitude in the dark current densities was observed between the samples. Two initial hypotheses were considered to explain this difference: (1) serial or parallel resistances introduced during process step, and (2) non-uniform Aluminium deposition on MBE growing process. In order to evaluate hypothesis (2), the activation energy for each sample was calculated using the measured temperature dependent low bias voltage conductance, and a specific simulation software the Aluminium concentration was estimated. As results, it was found a difference of 6.6% in the Ea and 5.5% in Al concentration between both samples, and up to 7% below the Al concentration previously designed. Additional details on the analysis will be presented.

Analytical Solution of the Radial Schrodinger Equation for the Modeling of Cylindrical Semiconductor Nanowire Transistors

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Increasingly sophisticated one-dimensional devices based on semiconductors nanostructures have attracted a great deal of interest for electronic and photonic applications. In fact, one-dimensional (1-D) devices have been fabricated by top-down as well as by bottom-up methods. It is now possible to fabricate nanowires which incorporate variations of doping and composition along their longitudinal length, with almost the same interface quality as in state-of-the-art MBE, and devices such as nanowire resonant tunneling diodes (RTDs) have already been demonstrated. Transistor action is obtained by placing an additional gate electrode, known as gate-all-around (GAA), surrounding the active region, which is composed by the nanowire superlattice of the RTT. The modeling of the electronic characteristics of nanowire resonant tunneling transistors is the focus of our research line. For use in TCAD software, the final goal is to obtain analytical, compact-modeling expressions for the current-voltage (I-V) characteristics as well as well related parameters, such as transcondutance and gate capacitance. In our proposed approach to obtain the I-V characteristics of the device, the longitudinal current transport across the wire is described by the transfer matrix method (TMM) and controlled by the gate action (allowed by the insertion of the GAA metal-oxide gate). Therefore, for an accurate model, it is crucial to solve the radial part of the Schrödinger equation and to compute the eigenenergies, taking into account that the Schottky contact at the gate creates a parabolic radial potential profile within the nanowire. In this communication, we analytically provide a closed-form solution to this problem, by the Nikiforov-Uvarov method (NU), well-known in relativity and nuclear physics but, to the best of our knowledge, never before used in semiconductor device modeling. Our results offer useful device design guidelines, indicating the doping range for which typical nanowire transistors are enhanced-mode, normally- off devices, to be turned on by applying a gate voltage close to the surface potential caused by Fermi-level pinning. In this case, the ground-state eigenenergy provided by the NU method approaches the value obtained in a free-standing nanowire.

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Asymmetric behavior of hole and electron mobilities in graphene devices due to hydrogen exposure

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Graphene, a single atomic layer of graphite has astonished the scientific community with its extraordinary physical and electrical properties [1,2]. Soon enough it was discovered that its electronic properties are strongly sensitive the environment and also by molecules assembled on its surface [3]. In this context, studies regarding the interaction between hydrogen (H2) and graphene devices have become particularly important due to the possibility of using graphene as a hydrogen storage material. Here, the electronic properties of monolayer graphene have been investigated (in situ) under the exposure of molecular hydrogen. Experiments during hydrogen adsorption and desorption at different conditions of hydrogen concentration and temperature (from room-temperature to up to 230°C) were performed. The field-effect transistor mobility of graphene is shown to be highly sensitive to hydrogen exposure demonstrating its direct effect on graphene charge scattering mechanisms. At 230 oC, the hole and electron mobilities react in an asymmetric way under hydrogen exposure, i.e, decreasing hole mobility while at the same time increasing electron mobility. Moreover, a change in the charge neutrality point towards more negative gate voltage is observed indicating an n-type doping effect. It is important to note that the whole process (adsorption and desorption of hydrogen) is fully reversible and only happens at 230 oC. This suggests that the process is thermally activated and might demonstrate the occurrence of dissociative H2 (H2 = 2H+ + 2e-). Thus, H+ might act as the scattering center and the extra electrons are responsible for the observed charge transfer. Further analysis to explain the influence of hydrogen on the electron and hole mobilities will be presented.

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Bound state of an impurity center and non-linear screening in a two-dimensional electron gas

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A uniform electron system is described theoretically by the so-called jellium model where electrons move freely in a positively charged uniform background of the same density. Many-body effects of an interacting electron system in simple metals and semiconductors can be well understood by reference to the homogeneous electron-gas model. The exchange and correlation effects of the electrons have been extensively studied. The correlation energies obtained by quantum Monte Carlo (QMC) calculations in three-dimensional (3D) and two-dimensional (2D) systems have been widely used in mean-field theory such as density functional theory for studying electronic structures of molecules and materials.

When an external point charge is introduced into a uniform electron system, it disturbs the electrons which in turn redistribute themselves so as to screen the charge at large distances. Screening reduces significantly the interaction range between charged particles in many processes. If the impurity center is of a positive charge $+e$, it can bind one electron forming an neutral impurity center D^0 or two electrons forming a negatively charged impurity center D^-. It is known that, at low-electron densities, the ground state of the impurity center is the D^- state. It is generally believed that this donor impurity can bound one electron only at high-electron density due to screening effects.

In this work, we study the bound states and screening effects of a donor impurity localized in a 2D electron layer using QMC. The ground-state energy and the charge distribution of the system are calculated in a wide range of the electron density ($r_s = 1$ to 30). The impurity-electron and electron-electron pair-correlation functions are obtained. We find that, though the binding energy decreases with increasing the electron density, the impurity center binds two electrons even at high density $r_s = 1$. We will discuss the electron-electron correlation effects, the nonlinear screening of the electron gas as well as the bound states of the impurity center in the 2D system.

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Carrier transfer in the optical recombination of quantum dots

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We report a study of dynamic effects detected in the time-resolved emission from quantum dot ensembles. Experimental procedures were developed to search for common behaviors found in quantum dot systems independently of their composition: three quantum dot samples were experimentally characterized. Systems with contrasting interdot coupling are compared and their sensitivity to the excitation energy is analyzed. Our experimental results are compared and contrasted with other results available in literature. The optical recombination time dependence on system parameters is derived and compared to the experimental findings. We discuss the effects of occupation of the ground state in both valence and conduction bands of semiconductor quantum dots in the dynamics of the system relaxation as well as the nonlinear effects.

Carriers Dynamics in Type-II Multilayer Structures: Stacked Quantum Dots and Quantum Posts

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Self-assembled quantum-dot (QD) systems have a large potential for device applications and offer several possibilities for fundamental physics investigation based on quantum effects. In particular, stacked QD structures are a powerful candidate for optical device applications due to their large active region. However, in type II systems, due to the spatial separation between electrons and holes, the electronic structure as well as the carrier dynamics are strongly dependent on the structure morphology and present very distinct optical properties as compared to type I structures [1]. In this work, we investigated the carrier dynamics in multi-layer InP/GaAs self-assembled quantum dots with a type II band-offset alignment. Optical measurements revealed remarkable results for structures with two distinct morphologies: weakly coupled stacked dots and coalescent vertical dots, usually called quantum posts. The long optical emission decay times observed by time-resolved photoluminescence experiments is an evidence of charge separation in our structures, in agreement with the predicted type II interfaces. This spatial separation of carriers plays a fundamental role on the carrier dynamics. For instance, the photoluminescence excitation results show that the transference of carriers from the wetting layers to the QDs, which is usually rather efficient in type I systems, show a particular different behavior in our samples. The results indicate that carrier transference between wetting layer and QDs in our structures is negligible at low temperatures, below $\sim$ 60 K. These results are discussed based on the type II character and the morphology of the stacked QDs.

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CdTe/HgTe (001) interface under pressure: an Ab initio study

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Recently a new class of materials with properties distinct from the usual ones have emerged. These materials, called Topological Insulators, have an energy gap in its bulk state while presenting conducting states at its surfaces/edges, which are topologically protected, with no scattering. They were theoretically predicted and later experimentally verified in some classes of materials as CdTe/HgTe interfaces, which are known as 2D Topological Insulators. In this work we have performed ab initio calculations on the CdTe/HgTe (001) interface using the VASP code. We used a 66 A thickness for each material composing the interface. A characterization of the edge states show textured spin states at the interface with a linear dispersion, forming what is known as the Dirac cone. We then study the influence of hydrostatic and biaxial external pressures leading to strains from -4% to 4% of the equilibrium lattice constants. The results show that the biaxial stress affects significantly the band structure of the heterostructure, following the expected tendencies of opening and closure of the band gap under compressive and tensile stress, respectively. The spin polarized states keep their linear dispersion only for the smallest tensile strains (1 and 2%), whereas for the compressive strains the linear dispersion is maintained only for the -1% strain value. On the other hand, hydrostatic pressures have only a very small influence on the band gap and the spin polarized states. Further, we have determined the valence, conduction and band gap deformation potentials of this system.

Chemical Reaction and Production of Cerium Oxide Films From Cerium Salts Using a Thermal Route: Thermogravimetry, Raman and X-ray Diffraction Analyses.

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In recent years the interest in CeO2-based devices has increased, mainly due to its catalytic properties, high dielectric constant (15 to 26) and wide band gap (3 - 4 eV), all of them highly desirable for the most recent developments in industrial processes and electronic devices such as storage capacitors and in photonics. The high dielectric constant together with its wide band gap and high transparency in the visible range makes it attractive for producing protective coatings. Other important uses of CeO2 are its application in photodegradation of polluting compounds, in water-gas shift reaction and three-way catalysts. Furthermore, it was shown that doping CeO2 with a small amount of Co generates films with high Curie temperature and giant magnetic moment, which can be explored in the emergent field of spintronics. In this work we report the chemical reaction describing the production of cerium dioxide from a thermal route, using as precursor reagents two different cerium salts: heptahydrated cerium chloride and hydrated cerium acetate. For the study of the thermal (pyrolytic) reaction, thermogravimetry-differential thermal analysis (TG-DTA) measurements were performed to the salts powder in the range from the room temperature (RT) to 900 °C. For complementation of the TG-DTA curves, Raman spectra and x-ray diffractograms for various intermediate stages of the thermal treatment were accomplished. After the achievement of the pyrolytic chemical reaction for both salts, we identified the optimal temperature to produce high quality CeO2. For cerium chloride it was up to 600 °C, whereas to cerium acetate it was up to 700 °C. With this, we grown ceria bulk films in this ideal temperature on Si(001)substrates using the drop casting deposition method and studied its optical and structural properties. Raman spectroscopy shows a strong and narrow peak at 464 cm-1 for both cerium chloride and cerium acetate films. XRD measures shows a polycrystalline pattern for both films, but with the narrowest width line in both analyses.

Circularly Polarized Photoluminescence as a Probe of the Spin Polarization in GaAs/AlGaAs Quantum Hall Bilayers

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We employ circular-polarization-resolved magneto-photoluminescence technique to probe the spin character of electron and hole states in a GaAs/AlGaAs strongly coupled double-quantum-well system. In the low magnetic field regime, degree of circular polarization and photoluminescence intensities of the lines associated with symmetric and antisymmetric electron states present clear out-of-phase oscillations between integer values of the filling factor v. These oscillations are caused by magnetic-field-induced changes in the population of occupied Landau levels near to the Fermi level of the system and may be understood in terms of a simple single-particle approach model [1]. In high-quantized magnetic field regime, at v below 4, the interaction effects lead to the magnetic-field-induced redistribution of charge over the Landau levels and produces the continuous formation of the charge density wave. Direct evidence for the symmetric-antisymmetric gap shrinkage at the filling factor $v = 3$ is reported. The observed interlayer charge exchange causes depolarization of the ferromagnetic ground state [2].

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Coherent manipulation of quantum dots in nanocavities

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The strong coupling between quantum dot and cavity has been subject of intense research in recent years. Many of these studies rely on understanding the avoided crossing seen in the emission spectral of such system, which is usually obtained by pumping the system with a laser above the band gap of the used semiconductor. The system is very rich and many other effects are expected with coherent resonant excitation.

In this work we study the effects of coherent laser in a system formed by an electrically tunable single quantum dot (QD) in a photonic crystal (PhC) nanocavity operating in the strong coupling regime of the light matter interaction. We model our system by assuming that the laser can create only one exciton in the QD, and that its energy is close to resonance with the cavity mode. We investigated the case where the energy of cavity mode is fixed and we vary both the energy of the QD and the frequency of the applied laser. In our simulations we solve numerically the time-dependent Schrödinger equation using a Runge-Kutta routine and we investigate the effect of a continuous and pulsed laser. First we used a weak continuous laser to map the absorption energy of the system using a procedure developed in this work. From the parameters we got we then simulated the effect of a pulsed laser. In our results we was able to show Rabi oscillations between many different state, for example, between the vacuum state (no excitation on the system) and the exciton state, vacuum and one exciton with one photon (a two photon process), and vacuum and one exciton with two photons (a three photon process). We also study the effect a pulsed laser in the population inversion for a cavity in the initial state of one exciton and a thermal distribution of 15 photons. In this case we were able to modify the revival observed in a typical coherent population inversion of QD-cavity system.

This work can give new insights for future experimental on QD-cavity system focusing coherent manipulation and quantum information processing.

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Comparing electronic and optical properties of wurtzite and zincblende free-standing nanowires

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In recent years, the advances of growth techniques allowed the fabrication of high quality single nanostructures with quantum confinement along the lateral directions. Although the radius of such structures is nanoscopic, varying from one to a few tens of nanometers, its length exceeds micrometers. These quasi one-dimensional structures are known as free-standing nanowires (FSNWs). The use of nanowires (NWs) in devices development has attracted great attention in the last decade since they can be used to increase the density of components in integrated nanocircuits [1]. Ever since, FSNWs have been proposed as building blocks for photo-detectors [2], sensors and field effect transistors. The applications involving FSNWs depends on its unique optical and electronic properties, e. g., the enhanced transport properties caused by the quasi one dimensional quantum confinement. However, the understanding of their optical properties still requires further theoretical effort. To achieve this knowledge various theoretical methods such as the k.p, tight-binding, density functional theory and pseudo-potential have been used to describe the electronic properties of semiconductor nanostructures. Among these, the k.p method is computationally the least costly considering the size of the modeling matrices involved. The aim of this study is to provide theoretical calculations of optical absorption power (AP) of InP FSNWs, comparing the results for two crystalline structures zincblende (ZB) and wurtzite (WZ) in equivalent growth directions: [111] for ZB and [0001] for WZ. The quantum confinement is addressed, analyzing the influence of energy level changes in narrowing the absorption spectra and as consequence, a parameter to tune of the electronic transitions. In this study, we use an approach that describes both crystalline structures in a single Hamiltonian using the k.p method, the envelop function formalism and the plane wave expansion [3]. AP calculation is done using the Fermi's Golden Rule [4] to provide us the rate of electronic transitions.

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Conductance quantum oscillations in quantum rings tuned by 2D quantum point contacts.

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In this report we study the influence of the Aharonov-Bohm (AB) and the Aharonov-Casher (AC) phases on the interference mechanism for a semiconducting quantum ring (QR), in the presence of Rashba type of spin orbit interaction. A particular subject of investigation, is the role of the upper- together with lower-arm 2D quantum point contact (QPC) to the transparency of the present device setup. We additionally consider another 2D QPCs, allocated symmetrically at the ring periphery, thus conforming a different lead-to-ring interface junctions [1]. Consistent with the AB-AC effects, expected conductance oscillations are obtained, and their behavior is analyzed as the opacity in the QPC changes. Being able to reproduce previously studied phenomena [1], we get a deeper inside into the Landau quasi-level spectrum of the proposed QR-setup with four QPCs, applying for that porpoise the transfer matrix formalism. It is shown that manipulating electrostatically the confinement strength at each QPC, as well as the AB and the AC phases, result into new harmonic patterns for the conductance. These phenomenology may be of utility to implement a novel way to modulate spin interference effects in semiconductor quantum rings, providing an appealing test-platform for spintronics applications [2]. A very perspective playground to detect changes in the resistance, is a QR-entanglement of layered films [3]. We predict that an array based on the present QR-device setup, could allow to clarify the significance of the topological parameters and the geometric phase contribution to the QR transparency.

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Control of spin photocurrents in diluted magnetic semiconductor heterostructure

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By employing the split-operator approach, we are able to determine the spin-dependence of the photocurrents extracted from ZnMnSe semiconductor heterostructures under the action of a static magnetic field of a few Tesla and under the action of an exciting THz field. To control the spin-polarization of the photocurrent, we found a particular structure arrangement of II-VI semiconductors that maximizes the difference between the spin dependence of both ground state wave functions and photocurrents. Our results show the existence of spectral domains in the THz range for which the spin polarization of the photocurrent is strongly sensitive to static biases applied in the growth direction of the structures. For such THz-photon frequencies, we demonstrate the possibility of effectively reversing the spin polarization controlled by an external bias and/or photon energy. The mechanism underlying these results can be understood in terms of the spin dependent profiles of the structures and the corresponding selection rules for the intraband transitions excited by the THz field.

Crossed persistent spin helices

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In Rashba-Dresselhaus quantum wells with tuned couplings spin-density wave patterns that are not susceptible to any type of spin-independent and/or electron-electron scatterings are possible. These long-lived persistent spin helices arise from the partial cancellation of the equal-strength Rashba and Dresselhaus spin-orbit terms which gives rise to a fixed spin quantization axis [1]. These robust excitations have been recently realized [2]. Two-subband quantum wells offer the possibility to obtain two distinctively gate-tunable Rashba couplings including their signs within a single system [3]. We have investigated the possibility for crossed persistent spin helices in realistic two-subband wells with orthogonal spin quantization axes for the first and second subband [4]. We find unique two-dimensional spin textures resulting from the coherent interference between the two crossed spin helices. We have performed a detailed self-consistent calculation of all relevant spin-orbit coupling parameters of our wells: i. e., the Rashba and Dresselhaus couplings within each subband and the corresponding intersubband couplings. We have also investigated the spin lifetime of the crossed spin helices. Interestingly, we find that for some parameter range the intersubband spin-orbit contributions can enhance the spin lifetimes. Transient spin grating spectroscopy [2] can, in principle, be used to probe these novel spin-density excitations. This work has been supported by: CNPq, FAPESP and PRP/USP (Q-NANO).

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Crossover of transverse momentum dependent effective valence-band offset for layered heterostructures: Pseudomorphic strain effects.

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The interplay of transverse-momentum-dependent effective *band offset* profile with heavy holes and light-holes, is detailed studied [1]. Thinking on optoelectronics and promising "spin-orbitonics" devices [2], highly specialized $III-V$ semiconductor binary-compound cases were considered, to present several new features in the metamorphosis of the rectangular effective *band offset* profile, in the presence of gradually increasing valence-band mixing. By means of a simple model, we evaluate the effect of a pseudomorphic strain on the effective *band offset* profile. Some $III-V$ unstrained semiconducting layered heterostructures, exhibit for light holes solely, an appealing crossover of quantum-well-like *versus* barrier-like roles, whenever the in-plane quasi-wavevector dependent kinetic energy, varies from low to large intensity. For strained heterostructures, we had detected this crossover for heavy holes only. We conclude that the effects of band mixing can not be universally neglected, due the relevance in the modelling of heterostructures that host more than one type of charge-carrier particles.

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Crystal structure and optical characterization of radial heterostructured GaAs/AlGaAs/GaAs nanowires

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Structural and optical properties of heterostructured GaAs/AlGaAs/GaAs core/inner shell/outer shell NWs are studied. Transmittance electron microscopy, CW and time-resolved photoluminescence as well as Raman scattering measurements unambiguously manifest to the presence of segments crystallized in zinc-blende and wurtzite phases, which spread to the shells. The effect of in-built electric field is to energetically separate optical transitions due to recombination of spatially separated electron-hole pairs. Four observed photoluminescence lines are assigned to the radiative recombination of photoexcited electrons confined in the center of the GaAs core and at the heteroboundary between the outer GaAs shell and the inner AlGaAs one with the holes localized at the heteroboundary between the core and the inner AlGaAs shell; both recombinations take place in zinc-blende and wurtzite phases. One additional photoluminescence line is attributed to the spatially indirect recombination between the electrons in zinc-blende and the holes in wurtzite phases. Band gap of the wurtzite phase and the band offsets between the zinc-blend and wurtzite structures are determined. A simple model, based on representation of the valence band structure using two levels, accounts well for the observed temperature dependence of the integrated photoluminescence intensities. The proposed double shell structure with tunneling transparent inner shell sets conditions for easy control of the emission energy of the heterostructured nanowires. In addition, time-resolved photoluminescence was employed to study electron-hole dynamics in radial heterostructured GaAs/AlGaAs/GaAs core/inner shell/outer shell nanowires. It was found that impurity random potential produces a red shift of the decay time maximum with respect to the photoluminescence peak energy.

DETERMINATION OF THE SPIN DIFFUSION LENGTH IN SILICON AT LOW TEMPERATURES

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The magnetoresistance of nanofabricated Ni/alumina/Si contacts was used to determine the spin diffusion length, when measured as a function of temperature and gap between contacts. The results are shown between 11 and 30 K. For temperatures above this upper limit no magnetoresistance effect was observed for the range of contact distances used (100 to 1500 nm). By fitting the data with an exponential, the diffusion condition, as a function of the gap, where the magnetoresistance takes place, we deduced the values of spin diffusion length and spin lifetime. The reduction of magnetoresistance at 30 K is consistent with the standard theory for spin injection from a metal to a semiconductor. This is more evident when measuring the resistances at different currents and voltages. The magnetoresistance increases when the currents or fields are increased.

Edge states in multiple topological mass domains

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Topological insulators (TIs) are a new class of materials that behave like metals and insulators at the same time. More specifically, More specifically, the surface states or edge states (2D case) of these materials are distributed continuously, i.e., they don't have an energy gap like metals, and the states in the occupied and empty bands in bulk are separated by a gap like in an ordinary insulator .The 2D topological insulating phase was first discovered in HgTe/CdTe quantum wells and its low-energy physics is described by the Bernevig-Hughes-Zhang model (1), in which the trivial or non-trivial insulating phase depends on the sign of the Dirac mass. In this work, we solve the BHZ model (using soft-wall boundary conditions) for a mass domain configuration, analyzing the effects on the edge states of a finite Dirac mass in the normal insulating region. We show that at the interface between a topological insulator (TI) and a normal insulator (NI), there is a strong dependence of the Dirac point on the ratio between the masses of the two different regions, TI and NI.

Effect of AlGaAs cladding on optical gain of GaAs/GaAs1-xBix/GaAs heterostructures

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Structural and optical properties of a GaAs1-xBix quantum well (QW) symmetrically cladded by a GaAs barrier with and without additional symmetrical confinement by the AlGaAs layers are studied and compared. It is shown that a GaAs/GaAs1-xBix/GaAs QW with Bi concentration of $\sim$ 4% and well width of $\sim$ 4 nm grown by molecular beam epitaxy demonstrates an efficient photoluminescence (PL) gain that becomes significantly thermally stabile if QW is cladded by AlGaAs layers. PL behavior, under changing the temperature from 10 K to 300 K and varying excitation intensity through seven orders by magnitude, is well described in terms of exciton dynamics included carrier capture in QW, thermal emission, and diffusion in the barrier. Understanding of these processes in dilute GaAs1-xBix QW structures lays a way to creation of highly efficient devices possessing reduced thermal sensitivity and threshold current.

Effective electron g-factor in III-V semiconductor quantum wells

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The renormalization of the electron g-factor due to the mesoscopic confining potential in a semiconductor quantum well (QW) was recently discussed within standard envelope-function approximation based on Kane's model for the bulk [1]. The theory agrees well with experiment and shows that the electron g-factor in III-V QWs is renormalized by a spin-orbit (SO) term with the same origin as the Rashba SO interaction term. However, specific solutions were given only for symmetric QWs [1]. Here we present and discuss the solution for the electron g-factor in the general case of asymmetric QWs. As in the symmetric case, a simple expression for the electron g-factor (as a function of the band and structure parameters) is obtained within first-order perturbation theory, but only with an special and auto-consistent choice of gauge for the external magnetic-field. Results for specific III-V triangular and flat-band asymmetric QWs are also discussed.

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Effects of a Mn-planar doping near a InGaAs/GaAs quantum well

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GaMnAs alloys have been extensively studied over the last decade due to their potential for spintronic applications. The main interest is to combine optical and electronic properties of the semiconductor with the magnetic ones to provide an additional interaction, such as carrier-ion exchange interaction, for novel devices development. Structures based on Mn delta-doped layers have been proposed as an alternative to attain Mn concentrations, in order to achieve the ferromagnetic phase at higher critical temperatures. We investigate a structure consisting of an (In,Ga)As/GaAs quantum well with a Mn delta-layer at the barrier. A key point is to find an optimal compromise between the distance between of the Mn layer and the quantum well, in order to achieve high-quality optical properties, and a high hole-gas mobility in the quantum well, preserving the coupling between the hole-gas and the Mn ions in order to maintain the magnetic ordering. We studied the effects of the nearby Mn ions on the optical properties and the spin dynamics of electrons confined in the quantum well. Photoluminescence and excitation photoluminescence measurements were carried out in series of InGaAs/GaAs quantum wells with different space layers thicknesses between the Mn-layer and the well, maintaining a constant amount of Mn. Hole-gas densities at the wells were estimated by the Stokes-shift energy from the e1-hh1 ground state transition. Beyond the expected transitions involving the confined states of the well, we observed a series of additional narrow absorption peaks in the excitation photoluminescence spectra, that become increasingly stronger for decreasing spacer layer thicknesses. Surprisingly, the polarization degree of the quantum well emission obtained from circular-polarized excitation at those peaks is identical to the polarization degree obtained from the quantum well transitions with similar energies. Furthermore, temperature effects on these sharp structures revealed weakly bounded states. We analyze the origin of these absorption peaks, their relation to the energy levels from the Mn delta-doping layer and the effects on the optical and magnetic properties of our structure.

Electric dipole spin resonance for inter-level transitions in double quantum dot

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The spin-orbit interaction (SOI) couples the motion of an electron and its spin. In this way an oscillating electric field can be used to act on the electron spin as a flipping mechanism. Transitions mixing spin states which are induced by ac electric fields via the SOI give rise to the so-called electric-dipole spin resonance. It has been shown both theoretically [1] and experimentally [2] that the spinflip rate mediated by SOI and ac electric fields is proportional to the applied magnetic field which is needed in order to break the Kramer degeneracy in the SOI Hamiltonian. In this work we investigate the solution of the time-dependent Schrödinger equation for two electrons in a double quantum dot, formed in a gated quantum wire under ac electric field.[3] Spinflip transitions induced by ac gates in the presence of SOI coupling are studied focusing on excitations allowing inter-orbital level transitions. The numerical method we used is based on the time-evolution of a two-electron state in the quantum dot potential and in the ac field. When the ac field frequency matches the energy of an allowed inter-level transition, the two-electron state is likely to make a transition, therefore mixing orbital states and also spin states via the SOI. Current generated from these stimulated ac-field transitions is also investigated since experiments rely on this information to access the spin states.[2]

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Electrical properties of TiO2 films deposited on Si/SiO2

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In this work, we investigate the electrical properties of TiO2 films for application on the development of photovoltaic devices. These materials have being investigated in the last 40 years because of its very special characteristics, such as relatively inexpensive, physical and chemical stability and low toxicity. However, some important parameters have not being fully studied, i.e., the energy gap cannot be controlled systematically. In addition, the devices developed using this material have presented low efficiency despite the different techniques that have been employed for the fabrication of structures based on TiO2. The films investigated in this work were prepared through the precursor solution of titanium and titanium with Zr. It was synthesize by polymeric precursor method, also called Pechini method. The films were deposited at Si/SiO2 substrate by spinning the deposition and it was calcined at 600 Graus Celcius for 2h. The electrical transport measurements were performed in the samples and electrical resistance curves were measured as a function of the temperature in the range of 300 K down to 7 K. The preliminary results have demonstrated that the electrical transport takes place via the film and shows that the substrate does not participate of the transport. We also intend to verify the effect of illumination in the electrical properties. In addition, the analysis performed on the electrical resistance curves using the activation energy method will allow us to determine the energy levels present in the material giving a general description of the transport mechanisms present in these films.

Electrically detected magnetic resonance modeling and fitting: a equivalent circuit approach

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Electrically Detected Magnetic Resonance (EDMR) is an interesting technique for studying spin-dependent processes and charge transport in real electronic devices under operating conditions. Recently published results have shown EDMR signals in phase quadrature for organic materials. Such signals have been attributed to the presence of distinct resonant species (electrons and holes) with different g-factor and/or different response times in the devices. However, this subject is still controversial and more studies are needed to better understand the phenomenon. In this work RC equivalent circuits were employed in order to model the EDMR signal and assess intrinsic features of the technique such as modulation effects and detection in phase quadrature. This approach allow fitting of the experimental EDMR spectrum of Alq3 based OLEDS. In addition, preliminaries results suggest that the signal at 90° in these systems can be attributed to the difference in response times of the resonant species present in the samples. The proposed equivalent circuit and the associated computational routine provide a powerful tool for experimental data processing as well as a better understanding of the EDMR spectrum for similar systems.

Electronic excitations in both rutile TiO_2 and SnO_2 bulk and (110) surfaces

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With the development of the TiO_2-based photo-active devices, such as hybrid photovoltaic ones with high power conversion efficiencies, the interest about the complete characterization of the TiO_2 surfaces was renewed. On the other side, SnO_2 is a compound for applications as transparent conducting electrodes, in solar cells as well as in other applications which attracted the interest of the scientific community for a better understanding of its electronic properties. However, despite the fact that the structural and electronic properties of both TiO_2 and SnO_2 surfaces have been extensively studied, little is known about the optical electronic excitations in these systems. So, in this work, we show, by using the by using the Time Dependent Density Functional Theory (TDDFT) within the Adiabatic Local Density Approximation for the exchange-correlation term, plane-wave description of the wave functions and the pseudopotential method (Abinit code), together with the slab-supercell description of the surfaces, the band structure and the electronic excitations of both rutile TiO_2 and SnO_2 bulk and (110) (1×1) surfaces. We have used the Troullier-Martins pseudopotentials, and the electronic excitations, as well as the optical absorption spectra, were obtained by the Casida approximation. In the surface calculations, we have used supercells build up of 7 atomic layers and a vacuum region equivalent of 10 atomic layers. We have analyzed their electronic structures and the theoretical optical absorption spectra. Our results are in good agreement with both the available theoretical and experimental data, whenever these comparisons were possible. Based on our obtained results, we describe the nature of the electronic transitions across the bandgap, which is an important feature for the concept of the new photovoltaic devices based on these materials, as well as the problems with the Casida approximation when applied to describe the SnO_2 nanostructures, one of the conclusions reached by this work.

Electronic Gap Modeling on Bilayer Graphene Nanoribbons

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We study electronic and magnetic properties of bilayer graphene nanoribbons with zigzag edges, using a Hubbard model and considering energy hopping up to second neighbor carbon atoms. The considered bilayer consists on a pair of graphene nanoribbons stacked in a Bernal configuration. The system is placed within two capacitor plates and we calculate the response on the transversal electric field following a mean field approximation. Similar to the case of a single graphene zigzag nanoribbon, the bilayer also presents localized edge-states in a non electron interacting picture and the density of states of the bilayer nanoribbons exhibit peaks at the Fermi energy. A spin-independent gap appear at the density of states when the Coulomb interaction is included into the theoretical picture. The system behaves ferromagnetically on the ribbon edges and antiferromagnetically over the width of the nanoribbons. The presence of a transversal electric field drastically changes this scenario, and as expected from the monolayer nanoribbon case, half metallicity is also observed for the bilayer nanoribbon systems. Differently from the single layer case, the gap dependence on the electric field intensity presents a well defined plateau for a particular range of electric values. We also present an analysis of tilted electric field in which biased graphene are considered as a limit case of zero transversal electric field.

Energy band gaps in Silicene and Germanene

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Graphene is a material that caught the attention of the scientific community due to its physical properties, especially their electronic properties. It is defined as a flat monolayer of carbon atoms, arranged in a hexagonal structure (honeycomb). More recently, first-principles calculations with optimized structure, phonon modes, and molecular dynamics at finite temperature, predicted that silicon and germanium can provide stable structures in honeycomb two-dimensional, similar to the graphene. More interesting is that their charge carriers also behave as fermions of Dirac massless, due to their bands that are traversed linearly at the Fermi level. In addition to these fundamental properties, nanoribbons of Si and Ge show remarkable electronic and magnetic properties, which are dependent on their size and orientation. These new structures offer interesting alternatives for the engineering of nanodevices using the silicon technology. In this work the band structure of Si and Ge sheets were obtained using the Density Functional Theory within the Projected Augment Waves method. In this work we show that without the inclusion of spin-orbit (SO) interactions, the states at the Fermi level present linear dispersions, behaving as really Dirac like states. However by including the SO interactions Silicene and Germanene present forbidden energy gap of 1.5 meV, and 24.0 meV, respectively. These systems with SO included present massive holes and electrons, and they are not any more Dirac like states. As the SO interactions are stronger than the Graphene, at the borders of Silicene and Germanene ribbon is expected topological protected Dirac states.

Energy transfer between multimodal- sized PbMnSe quantum dots embedded in a glass environment

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Semimagnetic Pb1-xMnxSe quantum dots were synthesized by fusion method in a glass matrix and characterized by optical absorption (OA), atomic/magnetic force microscopy (AFM/MFM), and photoluminescence techniques. MFM images strongly indicated the formation of Pb1-xMnxSe magnetic phases in the glass system. Quantum dot size was manipulated by tuning annealing time. It was shown that Mn2+ impurity affects nucleation, where Mn2+-doped samples present a redshift of the OA peak after a short annealing time and a blueshift after long annealing time compared to undoped PbSe NCs. This behavior was linked to the dependence of band-gap energy and the absorption selection rule on Mn2+ concentration. Photoluminescence in the Pb1-xMnxSe nanocrystals increases as the temperature rises up to a point and then decreases at higher temperatures. Anomalous increases in emission efficiency were analyzed by considering temperature induced carrier-transfer in semimagnetic Pb1-xMnxSe quantum dots nanocrystals of different sizes. Multimodal size distribution of the PbMnSe NCs was identified by spectral deconvolution of the PL spectra in Gaussian components. The temperature-dependent PL spectra show that the PL quenching temperature for different dot families is different. It was also shown that the coupling between QDs plays a key role in the unusual temperature dependence of the PL spectra. Larger QDs have lower energy transfer, which can be explained by the dependence of the surface states on the NC surface to volume ratio.

Excitonic and quasiparticle effects on optical properties of $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys: A first-principles study

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Optical properties of group-III nitrides and of their alloys are of increasing interest. This holds especially for the emission properties in the so called green gap. A deeper understanding of the interplay of clustering and composition fluctuations on the optical properties is needed. Random alloy and many-body theory of electron-electron interaction allow the modeling of corresponding spectra and can give an important contribution. In the present work, using many-body approaches for charged and neutral electronic excitations and a cluster expansion, the frequency-dependent dielectric function is computed for wurtzitic group-III nitride $In_xX_{1-x}N$ (X = Ga, Al) alloys for varying molar fraction *x*. Explicitly, we use the Vienna Ab-initio Simulation Package (VASP) to compute the quasiparticle electronic structure within an LDA+U+Δ approach and to construct the quasielectron-quasihole pair Hamiltonian to describe excitonic and local-field effects for each cluster. Two different cluster statistics are employed to perform the configurational averages for the optical functions. Based on the electronic structures, the BSE is solved and the optical absorption spectra, excitonic effects and macroscopic dielectric constants are computed for pseudobinary and binary end components. Comparing the resulting absorption peak positions and intensities (as a function of composition) to experimental data provides deep insight into the distribution of the group-III cations in the alloys.

Exploring transport properties in quantum dot chains

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With a variety of potential applications, the interest on the properties of low dimensional systems such as quantum wires (QWRs) and coupled quantum dots (QDs) has grown. Thus, progress has been attained in nano-scale architectures where, by using molecular-beam-epitaxy and skillful strain engineering, systems of aligned QDs into quantum dot chains (QDCs), were successfully synthesized. These samples allowed the study of electron transport through InGaAs QDCs with varying doping concentration through remote doping in the GaAs barrier. Hall bar structures were used for the electrical characterization that enabled the mobility as a function of temperature and the anisotropic conductance (along and across the QDCs). We contrasted these results with 1D hopping models. The peculiar effect of changing the relative position of the Fermi level is discussed. The nature of the carrier transport is complex due to availability of states of different dimensionality. The presence of 0D states shapes the anisotropic response in these systems. At low temperatures, the experimental response of all samples deviates from the Mott's law of conduction.

Extended DFT+U+V method with on-site and inter-site electronic interactions

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In this work we introduce a generalization of the popular DFT + U method based on the extended Hubbard model that includes on-site and inter-site electronic interactions. The novel corrective Hamiltonian is designed to study systems for which electrons are not completely localized on atomic states (according to the general scheme of Mott localization) and hybridization between orbitals from different sites plays an important role. The application of the extended functional to archetypal Mott-charge-transfer (NiO) and covalently bonded insulators (Si and GaAs) demonstrates its accuracy and versatility and the possibility to obtain a unifying and equally accurate description for a broad range of very diverse systems.

Fano resonance in GaAs photonic crystals

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A photonic crystal is a structure with a periodic variation of the index of refraction that allows one to control light propagation. These structures have been attracting ever increasing attention over the last few decades, due to their many technological applications and also due to their use as a tool to study fundamental physics phenomena such as Fano resonance, strong and weak coupling between light and matter and quantum dot induced transparency. Two dimensional photonic cavities fabricated by patterning a slab of material are relatively easy to make and permit one to obtain high quality factors. In this work, we investigate by reflectivity measurements a so-called L3 cavity, i.e., a line of three holes missing from an hexagonal lattice of air holes in a GaAs membrane. We observe Fano resonance in the reflectivity spectra, due to the interference between the light scattered from the periodic photonic crystal pattern and that scattered by the photonic modes. The effect of the polarization of the incident light is shown to be a tool to tune the Fano resonance. We also discuss the effect of scattering from self-assembled quantum dots that are embedded in the photonic crystal slab.

First principles study of Graphene, Boron Nitride and hybrid C/BN Nanoribbons

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Carbon nanomaterials , like nanotubes (NTs), fullerenes, graphene and nanoribbons (NRs), have great interest in material science because of the novel low-dimensional properties. Graphene is a single planar sheet compound of carbon atoms with the honeycomb structure. Similar to graphite it is a semimetal with a zero energy band gap. It was firstly obtained by Novoselov et al, since then has emerged as a candidate to replace the silicon in the development of new electronic devices. However, a limitation in the use of graphene is the absence of a band gap, which prevents any efficient flow of electronic current. One way to around this problem is the fabrication of graphene nanoribbons (GNRs) which have a band gap due the edge states. The GNRs have different edges terminations, typically zigzag or armchair. For the zigzag GNRs a spin polarization of the two edges states is observed with the anti-ferromagnetic (AFM) phase been semiconductor and more stable than the semi-metal ferromagnetic (FM) one. Otherwise, the armchair GNRs is a nonmagnetic semiconductor. The hexagonal boron nitride (h-BN) presents similar structure than graphite and also is able to form two-dimensional nanostructures, like sheets and nanoribbons (BNNRs) with a wide energy band gap. The hybrids C/BN nanoribbons (CBNNRs), where carbon and boron nitride are mixed in different stoichiometry have intermediate properties between the GNRs and BNRs and the electronic properties are show to be dependent of the stoichiometry. In this work, using first principles calculations based on the Spin Polarized Density Functional Theory (DFT) with the Generalized Gradient Approximation (GGA) for the exchange-correlation term as implemented in the SIESTA code, we study the structural, energetic and electronic properties of the hybrids C/BN NRs with different edges terminations. The dangling bonds of the edge states are saturated with different atoms H, F, Cl, S, O and Na) or molecules (OH, H2, O2, NOx, SOx, COx). We observe that their electronic and magnetic properties are dependent of the edge terminations. We obtain semiconductor with different band gap, metallic and half metallic systems.

First-principles calculations for group III impurities doping PbSe and PbTe: bulk and nanowire

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Fully relativistic calculations are used to perform a systematic investigaton on the energetic stability and electronic properties of group III elements (Al, Ga, In, and Tl) doped PbSe and PbTe: bulk and nanowire (NW). The calculations are based in the framework of the Density Functional Theory (DFT) with the General Gradient Approximation (GGA) for the exchange-correlation term. The valence and core electrons interactions are describe through the Projected Augmented Wave (PAW) method as implemented in the VASP code. Our results show that group III impurities have lower formations energies in the NWs as compared to the bulk ones. In addition we observe a trend for the impurities migrate to the surface of the NWs. In the bulk of PbSe and PbTe, Al and In are donor impurities while Ga and Tl are acceptor ones. For the NWs, the same trend is obtained for Al and Tl, whereas Ga and In give rise to deep electronic levels within the band gap. A two-level model based on the interaction between the impurity state and the host crystalline field explains the unexpected electronic properties of group III impurities doped PbSe and PbTe. This model agree with the projected density of states (pDOS) and help us to understand the unexpected n-type character of some group III impurities doped lead chalcogenides.

Franck-Condon Analysis: An approach to probe thermal activated process and conjugation length in stretched organic semiconductor thin films

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Photophysics processes in conjugated polymer are closely related with the molecular segments conformation. Conjugated polymers thin films has shown an intrinsic anisotropy due to the molecular segments conformation making this materials attractive in photophysics studies by its polarized emission when stimulated by light or biased. In this work, we correlated the photoluminescence spectra of a PFO derivative polymer thin films, namely poly(9,9-dioctylfluorenyl-2,7-diyl) end capped with dimethylphenyl with the molecular anisotropy. PFO thin films were spun casting over Teflon substrate and then mechanically stretched. Mechanically stretched thin films undergo a molecular rearrangement process inducing polarized light emission predominantly in the stretching direction. The photoluminescence spectra are composed by emission of different species, namely isolated and aggregate species. Measurements of photoluminescence excitation (PLE) have demonstrated the PL spectrum consists of a spectral overlapping of these two emitting species. By Franck-Condon analysis the PL spectra were fitted assigning to the active phonon mode to each emitting species. The fitting results show an increasing of the Huang-Rhys parameter for stretched samples indicating an increasing in the conjugation length of these films. Yet the half Gaussian bandwidth of fitted PL spectrum showed temperature dependence (starting at T = 280 K) to the active phonon mode corresponding to C9 carbon polyfluorene. These thermally activated process that corresponds to the beginning of the molecular dynamics of the polyfluorene side chains, known as transition beta. By an Arrhenius plot was possible determine the activation energy of this process, corresponding to 0,23 $\pm$ 0,04 eV, as previously reported in the literature by dielectric relaxation measurements.

Genetic Algorithm coupled to a Multi-Grid method and the Graph Theory to the determination of the equilibrium structure of atomic clusters

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The last twenty years have seen great efforts to understand the physical and chemical properties atomic clusters. This has been driven by some factors , like: (i) the great potential for applications of clusters in areas such as electronics , catalysis and hydrogen storage, for example; (ii) the agreement that clusters can be used as building blocks for new materials; (iii) the fact that their properties depend directly on the number of atoms in the cluster. In order to determine the cluster properties, it is crucial to know their equilibrium geometries. The search for the equilibrium geometries of clusters clusters is known to be a formidable theoretical challenge due to the large quantity os local minima that even particles os less than ten atoms can have. Among all alternative methods devised to search for the minimum energy configuration of a cluster, we will be focusing our study on the use of a genetic algorithm, which uses operators such as crossover and mutation, coupled with multi-grid techniques and the spectral graph theory (via SPRINT coordinates (PIETRUCCI AND ANDREONI, 2011)) to determine the equilibrium structures of argon clusters with 13, 55 and 147 atoms. The total energy of the argon clusters are calculated through the Lennard-Jones potential. The efficiency of the proposed approach is compared with the performance of the same genetic algorithm (same rates of crossover, mutation and elitism, population size, etc) that, however, do not use the spatial discretization (via multi-grid scheme) or the individuals selection of the population according to its topology (via spectral graph theory).

Going small: The effects of confinement

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It is known that many new physical effects and properties arise in the nano-scale, when the whole system is a couple of nanometers wide, so that even electrons start to feel confined. In this presentation we will show two different effects that appear in the electrical and optical spectra of the TiO2 oxide due to confinement.

We will present state-of-the-art, many-body perturbation theory GW calculations, for TiO2 anatase (101) slabs with varying number of layers, of the order of 1-2 nm wide [1]. We use for that ab initio approach based on the plane-waves, pseudo-potential methodology [2,3]. At this many-electron level, we can see the opening of the electronic fundamental gap as the width of the system decreases, an effect that is barely detected using Density Functional Theory, even when hybrid functionals are employed.

On another direction is the effect of confinement on optical properties: for that we focus on 4-layer slabs and compare to the crystalline structure, using many-body configuration-interaction CIS calculations with the MSINDO semi-empirical parametrization [4], adapted to periodic systems through the cyclic cluster approach. The lower-energy excitations display a clear surface-state character, as opposed to the highly delocalized excitons in the crystalline system (as also the higher-energy peaks in the slab). The surface exciton is quite localized, electron and hole interact strongly, resulting in a decrease of the optical gap. This effect will be more relevant for nanostructures, due to the higher surface/volume proportion.

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Growth of submonolayer InAs quantum dots for infrared photodetection

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Self-assembled InAs/GaAs quantum dots (QDs), directly obtained by epitaxial techniques in the Stranski-Krastnov growth mode, already found several technological applications but still suffer from their low areal density, high aspect ratio and lack of control during epitaxy. These features are extremely harmful to any application in the field of infrared photodetection and need to be overcome in order for such devices to reach their theoretical performance [1]. Recently, submonolayer quantum dots (SMLQDs) were proposed [2] and are expected to solve most of those issues. The main idea is to deposit only a fraction of a monolayer of InAs material (generally 30 to 70 %) in order to nucleate a high density of two-dimensional (2d) islands on the GaAs substrate, and then to cover those islands with a specific number of GaAs monolayers. By repeating that sequence as many times as necessary, a very high density (up to 1E12 cm-2) of InGaAs QDs of any desired height and composition can be obtained in a highly controllable way. Indeed, due to the elastic strain present in the InAs/GaAs system (which results from the difference of lattice parameter between InAs and GaAs), the islands from the next InAs submonolayers will have a tendency to nucleate above the ones of the previous InAs layers, thus forming stacks of electronically coupled 2d InAs islands, separated by GaAs material, that will behave as InGaAs quantum dots. Another feature of such structures is that they have no wetting layer, unlike usual QDs, and therefore accumulate less elastic energy in the system.

After choosing carefully the growth conditions, SMLQDs were successfully grown by molecular beam epitaxy (MBE) and showed an extremely strong and narrow photoluminescence spectrum (full width at half maximum around 10 meV), even above liquid-nitrogen temperature. When illuminated at 45° by a polarized infrared radiation, a QDIP grown with that kind of QDs showed a stronger lateral confinement than in usual QDIPs. Experimental results about these structures and related devices will be discussed.

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Heat Transport in GaN

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It is presented a generalized Hydro-Thermodynamics (called Mesoscopic Hydro-Thermodynamics MHT) of phonons in semiconductors, driven away from equilibrium by external forces, derived by the method of moments from a generalized Peierls-Boltzmann kinetic equation built in the framework of a Non-Equilibrium Statistical Ensemble Formalism. The resulting MHT involves the enormous set of coupled evolution equations for the densities of the quasi-particles (phonons) and their energy together with their fluxes of all orders. The handling of them requires the introduction of a contraction of description what defines MHT's of different orders. We illustrate the matter analyzing heat transport by phonons in GaN within the framework of a MHT of first order to obtain a generalized Guyer-Krumhansl equation from which it is analyzed the effect of geometry on the heat transport. It is described the influence of size (from bulk to nanometric scales) on the reduction of the thermal conductivity and the improving of the figure of merit of thermoelectric devices. It is specified a cylindrical geometry in samples of GaN, with varying radius R in the macro to nano-scales, centering the attention on the study of the thermal conductivity and its influence on the figure-of-merit in thermoelectric devices. The thermal conductivity is strongly dependent on the ratio of the cylinder radius to a characteristic length L, i.e., on R/L, given approximately by the velocity of sound time a kind of relaxation time (energy Maxwell time) resulting to be in the order of hundreds of nanometers. The contribution associated with L in the evolution equation for the flux arises from the use of a MHT of order 1, being inexistent in stand linear hydrodynamics (it consists in a Burnett-type term, quadratic in the wavenumber). From the performed full analysis, it was identified the particular phenomenon that there follows a steep decrease, of orders magnitude, after values of the radius R are equal and smaller than L, and therefore the thermoelectric figure-of-merit largely improve. The phenomenon could be interpreted as a consequence of the system entering in a ballistic-like scattering regime.

Helical states in curved bilayer graphene

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We study spin effects of quantum wires formed in bilayer graphene by electrostatic confinement. With a proper choice of the confinement direction, we show that in the presence of magnetic field, spin orbit interaction induced by curvature, and intervalley scattering, bound states emerge that are helical. The localization length of these helical states can be modulated by the gate voltage which enables the control of the tunnel coupling between two parallel wires. Allowing for proximity effect via an s-wave superconductor, we show that the helical modes give rise to Majorana fermions in bilayer graphene.

High-energy emission band from EuTe and PbEuTe alloys

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EuTe is a magnetic semiconductor that presents a band gap energy in the visible range and a remarkable exchange interaction between electrons in the conduction band and the magnetic ions, Eu. Therefore, it is a promise candidate for spintronic applications. The near-gap emission band from EuTe epitaxial films usually known as MX (1.92 eV) was attributed to an excitonic recombination associated to magnetic polarons involving electrons at the X-point conduction band minimum and holes at the 4f-energy levels of Eu2+ above the valence band maximum [1]. In this work, we report on the properties of this magnetic-polaron emission and an additional higher-energy emission band observed for high excitation intensity conditions [2]. These emission bands were investigated in epitaxial films of both EuTe and PbEuTe with low Pb concentration (≤ 0.05) at different temperatures, excitation intensities and magnetic fields, as well as their time evolution under pulsed excitation. The high-energy emission band is, likewise the MX band, strongly dependent on the magnetic field, while it presents a much shorter lifetime as compared to MX. We therefore attribute this novel band to an excitonic recombination involving a higher-energy conduction band valley. In the case of PbEuTe alloys, the MX band reduces its intensity as the Pb composition increases, but the additional band remains relatively strong and splits in several emission lines in the presence of high magnetic fields. Moreover, a broad emission band appears at 1.8 eV [3], which is attributed to a recombination involving deep levels, probably related to Pb atoms located at the original Eu sites.

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InAsP/GaAs self-assembled quantum dots with vertical and in-plane alignment

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Recently it was demonstrated that it is possible to grow a layer of InP quantum dots (QDs) arranged in a square lattice over the surface of an InGaP layer [1]. This is a bottom up strategy to fabricate three-dimensional, ordered arrays of quantum dots. This new technology relies on the adequate tailoring of an InGaP layer, inducing a vertical compositional modulation that pinpoints the nucleation of QDs in a square arrangement. It is possible to use this first plane of nanostructures as a seed for achieving an ordered, 3D lattice of InAsP/GaAs QDs. In this work we report on a photoluminescence (PL) study that identifies the optical signature of the InGaP compositional modulation; in the sequence we describe the growth of InAsP/GaAs quantum dots [2] (randomly distributed in the plane in the first approach), we discuss the effective mass calculations that estimate the effect of the GaAs separation layer thickness on the QD electronic states, and we present our current efforts towards the stacking of layers of InAsP QDs. Samples were grown by Chemical Beam Epitaxy on GaAs substrates. PL measurements were performed in a closed-circuit He Cryostat with temperatures ranging from 10 to 300 K, using a 532 nm solid-state laser as excitation source. A careful analysis of the optical experiments allows us to identify the signature of the compositional modulation, since the PL energy vs temperature curves present a "s-shaped" evolution of PL line as a function of temperature for samples where InGaP layer presents this effect. Control samples, without any compositional modulation, display the usual, monotonical Varshni-like behavior instead. This "s-shaped" curve is characteristics of the potential flutuations in the InGaP layer that leads to the in-plane square arrangement of QDs. In order to guide the growth of stacked planes of InAsP QDs, we performed a simple effective-mass calculation comparing 3, 4, 5, and 6 QDs separated by GaAs barriers (spacing layers) varying from 2 to 15 nm. A configuration with three QD planes seems to be the most suitable to experimentally observe the effect of barrier width on the QD electronic states. Finally, we discuss our current results on the QD stacking.

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Influence of Mn dopants on the optical properties of Er-doped SrAl2O4

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The optical properties of rare-earth-doped alkaline earth aluminates have attracted much attention in the last years due to their high quantum efficiency, long-afterglow phosphorescence and chemical stability. However, there is a lack of understanding about the nature of the rare earth ions traps and the mechanisms which could activate and improve such emission centers in these materials. In this work, we have investigated a set of samples prepared by solid state reaction ranging from pure SrAl2O4 (as a reference), to SrAl2O4:Mn, SrAl2O4:Er and SrAl2O4:Mn:Er. Our samples were characterized by photoluminescence (PL), SQUID magnetization, Raman and optical absorption techniques. We have used the co-doping of Mn in order to improve the optical emission intensity of the transition I13/2 – I15/2 of erbium ions in SrAl2O4. The magnetic properties show that the Er co-doping results in a paramagnetic phase for of the samples. The PL spectra were obtained in the visible-infrared region using as excitation source the lines L1= 325 nm and L2 = 422 nm of HeCd laser at 300 K. Under L1 excitation, we have observed that the introduction of such dopants clearly influences an emission band in the visible range at 2.7eV and causes a strong blue shift to 3.0eV for all samples. The intensity of the emission 3.0eV is suppressed when both ions are in the matrix. As a result, the emission in IR-range is increased by 4 times whereas under L2 excitation the observed emission intensities are inverted. Our results may be explained by an energy transfer mechanism from the host matrix to Mn and then onwards to the Er sites. Although this implies a two step process, the observations are consistent with an improvement in overall efficiency.

Interaction of InAs QDs with Surface Plasmon Polaritons

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In the last years Plasmonics has become an important research area, whose main subject is to study the propagation of electromagnetic waves tightly confined to the interface between a metal and a dielectric, the Surface Plasmon Polartitons (SPPs). These surface waves have the ability to confine high electromagnetic fields in small regions near the interface between the two media, and these fields interact strongly with free charges along the metal, what generates electronic surface waves that propagate along the interface. In the meantime, efforts have been made to study QDs in the strong coupling regime, due to its high photon emission efficiency because of the quantum confinement in three dimensions. The high electromagnetic fields present in patterned plasmonic nanostructures can be used to excite QDs grown near these interfaces, and drive non-linear effects in the SPP-QD interaction. Our objective here is to study the interaction between SPPs in a plasmonic nanostructure and InAs quantum dots grown by Molecular Beam Epitaxy (MBE), in Stranski-Krastanov growth mode. The QDs were grown in a GaAs substrate and covered by a thin gold layer. A set of parallel slits were fabricated in the gold layer by a Focused Ion Beam (FIB) technique. In the work we present photoluminescence measurements of the samples obtained with and without slits as well as FDTD simulations of the given systems for transmitted light.

Interband absorption and light polarization in polytypical InP superlattices

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Polytypical superlattices with crystal phase mixing are nowadays experimentally achievable in III-V semiconductor nanowhiskers (NWs) [1]. Tuning growth conditions, such as temperature, diameter and III/V ratio, allows the assembly of high quality samples with well defined wurtzite (WZ) and zinc-blende (ZB) segments. This high degree of control during the NW growth opens new possibilities of band gap engineering, important in the building of novel devices and, also, in the understanding of fundamental concepts of electronic and optical properties. Despite the great number of experimental studies in polytypical superlattices, the effects of strain and polarization that can appear in these systems are not fully understood. Even though there is one kind of material in the structure, there can be some lattice mismatch between the two crystal phases leading to strain and piezoelectric polarization effects [2]. Also, WZ compounds exhibit spontaneous polarization effects due to relative displacements of the cations and anions. Such strain and polarization effects have great influence in the band structure and optical properties of semiconductor systems and should be taken into account. In this study, we analyze theoretically the strain and polarization effects on the band structure and interband absorption of WZ/ZB InP superlattices. The polytypical k.p approach [3] is applied to obtain the electronic structure and the resulting states are used to calculate the absorption spectrum, based on the semi-classical light-matter interaction hamiltonian. Besides the strain and polarization effects, different lengths of WZ and ZB regions are also considered in the calculations. The absorption spectrum in these different regimes (larger WZ segments or larger ZB segments) are compared to the bulk case in order to understand how crystal phase affects the light polarization. In summary, the results obtained from our study can improve the present knowledge of polytypical superlattices, especially how strain, polarization and length effects modify the interband transitions and light polarization.

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Interpolating meshfree method applied in quantum well and quantum dot infrared photodetectors

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The development of nanostructured infrared sensors based on quantum wells (QWIPs) and quantum dots (QDIPs) have received considerable attention of some research institutions and Universities in Brazil. QWIPs present several advantages over "bulk" intrinsic sensors, such as better selectivity, high yield, low cost and more thermal stability. QDIPs provide, theoretically, additional advantages over QWIPs, such as, lower dark current, higher operating temperatures and detection of normal radiation incidence. Different of bulk sensors, QWIPs and QDIPs consist of a sequence of layers of different semiconductor alloys. In these sensors, the parameters of interest are determined by the physical size of each layer and by the properties of the materials used in the heterostructure. CAD/CAE software tools are used to assist the design of these devices. In these software programs, numerical methods are applied to solve the equations that govern the physical phenomenon involved. The Interpolating Element-Free Galerkin Method (IEFGM) was proposed as an alternative to existing methods based on domain discretization, providing arbitrarily continuous solution not dependent of an explicit mesh. Being a relatively new method, the literature lacks information on the behavior of IEFGM in various applications. In this work the IEFGM is applied to solve both the one-dimensional and the bi-dimensional Schrodinger equation obtaining the energy levels and wave functions in quantum wells and quantum dots nanostructures. For quantum dots the Schrodinger equation is written in cylindrical coordinates. Solutions for nanostructures presented in the Literature were compared with our IEFGM solutions. The comparison was used to evaluate the performance of the method and to set appropriate values for certain IEFGM inherent parameters. This phase of the study allowed the definition of set of parameters for which the IEFGM solutions were maintained within an acceptable margin of error when compared to the Finite Element Method (FEM) and the Literature solutions. Having defined the parameters, structures with a quantum dot immersed in quantum wells were evaluated. In these cases, solutions obtained by FEM were also used for comparison purpose. The results obtained for these structures show that additional studies have to be carried out in order to determine adequate range of IEFGM parameters to obtain robust results, independent of the considered heterostructure and of the users' skill.

Investigation of luminescence spectra in p-type GaAs/InGaAsN SLs

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In the past few years, the dilute nitride system, InGaAsN, is proposed as a good candidate for several device applications. InGaAsN is considered a promising material for laser devices, telecommunication systems operating in a wavelength range of 1300-1500 nm and high-efficiency multijunction solar cells. However, the incorporation of relatively large concentrations of In and N into GaAs, which is necessary for obtaining structures with active regions operating in a wavelength range up to 1550 nm. Besides, the strain can be minimized since the opposite effect of In and N on the lattice constant enables lattice matching of InGaAsN on GaAs. However, despite their great potential for applications, the understanding of their physical properties is rather incomplete. In particular, the dominant mechanisms of light emission in these alloys and their dependence on the nitrogen composition are not well established. Such information is crucial not only for a better understanding of the optical properties of the nitrogen containing III-V alloys, but also for a better technological control of alloy formation and optimization light emission efficiency. Another point concerns to investigation in p-type doping in InGaAsN. This is of great importance since, for example, can improve the transport in HBT (Heterojunction Bipolar Transistors) devices. In this work we report on theoretical luminescence spectra calculations for p-doped GaAs/InGaAsN quantum wells and superlattices. The calculations are performed within the k.p method by solving the full 8x8 Kane Hamiltonian, generalized to treat different materials. Strain effects due the lattice mismatch between InGaAsN and GaAs are taken into account. By varying the acceptor concentration we analyze the effect of exchange-correlation, which plays an important role in profile potential and electronic transition. These results can explain several important aspects about optical properties in these systems.

Investigation of optical and electronic properties in SMDs based on group III - V

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Diluted magnetic semiconductors (DMSs) are recently the most active area of research due to development of spintronic devices, which is related to their magnetic and transport properties. The DMSs are produced introducing magnetic elements in non-magnetic semiconductors; the principle is the injection of spin-polarized carriers. The materials commonly studied in the literature are II – VI and III – V group, which are doped with transition metals. Experimental data indicate Curie temperature as high as 110 K for elements of III – TM – V group, GaAs:TM, where TM means transition metals.The quaternary alloy magnetic semiconductor InGaAs:Mn has many potential advantages that cannot be realized by ternary alloy magnetic semiconductors. For instance, the band gap energy, easy magnetization axis, and band structure can be controlled by changing the In content of InGaAs:Mn. It has been reported that strained InGaAs:Mn or InGaAs layers, using post-growth anneling at temperatures near the growth temperature, into the magnetic active GaAs:Mn can increase the TC above 100 K. In this work, we use the method k.p, within of Kane model 8 x 8. The solution is obtained self-consistently by the solution of the effective mass equation together with the Poisson equation. In this system we introduce the strain and exchange-correlation effects, which should be considered in the calculations. We investigate the behavior of system GaAs/(n x InGaAs/InGaAs: TM), where n is the number of magnetic layers. In particularly, we study the spin charge density, the polarization and theoretical photoluminescence in these systems as a function of the variation of In and Mn contents. We analyze the mobility in the non-magnetic and magnetic layers with the polarization due to the strain effects. Our results may provide a realist description for optical and transport properties in these structures.

Investigation of the vertical transport in cubic p-type superlattices

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Semiconductor superlattices (SLs), consisting either of a periodic sequence of thin layers of two or more different semiconductor materials, have been extensively studied from different points of view in past years. There are several reports on the transport properties of electrons in SLs, mainly due to the predicted negative differential conductance and the Bloch oscillations. In order to obtain a higher conductivity in these systems, it is necessary the presence of electron/hole dispersions in the minibands for carriers. However, an important part of these studies, theoretical and experimental, is devoted to only n-type systems, and very little has been reported in the literature concerning p-type materials. Besides, highly conductive p-type layers are of crucial importance for various electronic and optoelectronic devices as light-emitting diodes (LEDs), operating in the visible and ultraviolet spectra. In this work we extend our previous studies on the behavior of the electrical conductivity and plasma frequency in p-type SLs, for $ZnSe/ZnTe$, $Si/SiGe$ and cubic (c) $AlInGaN$ SLs. The calculations are performed within the $\vec{k} \cdot \vec{p}$ method by means of solving self-consistently a 6 $\times$ 6 Luttinger Hamiltonian together with the Poisson equation in a plane wave representation, including exchange-correlation effects within the local density approximation. The conductivity σ as a function of the acceptor donor concentration (N_A), is determined by using the quasi-classical transport theory based on Boltzmann's equation within the relaxation time approximation. The plasma frequency ω_p can be written in terms of σ. Our results indicate the constant increase of σ and ω_p due to exchange-correlation effects, effective masses and mainly the Fermi position inside the minibands. However, comparing all systems we observe an important contribution to conductivity from second occupied miniband given by light holes in $ZnSe/ZnTe$ and $Si/SiGe$ and split-off holes in $c-AlInGaN$ SLs. We also confirm that the more efficient systems with high conductivity are those based on II-VI and IV groups. Additionally, these results can give important information and clues towards its use a guide in experimental data for developing new electronic structures for device applications.

Ionization Potential and fundamental band gap of organic semiconductors: a many-body based approach

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Semiconducting conjugated polymers have attracted considerable interest as active organic materials for optoelectronic applications. The suitability of such organic semiconductors for device fabrication relies on quantitative understanding and control of key properties. Of particular relevance are the fundamental gap (Eg) and ionization potential (IP). While DFT calculations based on total energy differences have been successfully applied to estimate IPs of small molecules, they fail for properties of long conjugated systems. Indeed, the predictive ability of standard DFT with respect to spectroscopic properties is often limited, however a proper treatment of the electronic excitations through many-body approaches is still prohibitive for complex organic materials. Hybrid functionals that mix a fraction (a) of nonlocal exact exchange (EX) with the semilocal counterpart represent a good alternative, although the ideal amount of EX is usually system dependent. Here we adopt a non-empirical scheme based on the G0W0 approximation to identify the optimum α-value for the PBE hybrid functional, for which the self-energy correction to the generalized Kohn-Sham highest occupied molecular orbital (HOMO) is minimized [1]. Based on this strategy we study the size dependence of the electronic properties in the family of 1D conjugated acetylene oligomers, reaching to trans-polyacetylene (TPA). For small molecules (n=1-4), our calculations show that the size dependent optimal EX fraction incorporated in PBEh accurately reproduces IPs from experimental gas phase data, although no direct constraint has been applied to fit experimental data. Due to the similar nature of the frontier orbitals in TPA, the HOMO-LUMO gap calculated with our optimized PBEh is also in good agreement with the fundamental gap of G0W0 calculation. Furthermore, we note that optimal a-value varies very slightly with chain length, from a=0.85 for ethylene (n=1) up to a=0.75 extrapolated for an isolated TPA chain. The accuracy of the eigenvalue spectra of the optimal PBEh is examined for an alkyl-terminated trans-acetylene oligomer (n=7) by a direct comparison with photoemission experiments. Our optimally tuned PBEh is therefore suitable for calculating band structures of semiconducting polymers employing orbital energies.

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k.p Parameters of III-V Wurtzite Semiconductors From First-Principles Calculations

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Band structure calculations play a fundamental role in solid-state physics and quantum chemistry. One successful approach for this calculations is the first-principles, or "ab initio", method based on the Density Functional Theory (DFT) [1]. This DFT framework uses a self-consistent calculation to find solutions in the Kohn-Sham equations, the ones that describe the interacting electrons in the material. Although this "ab initio" approaches works fine for bulk systems, the calculations for confined structures, such as quantum wells, wires and dots, require a large number of atoms, considerably increasing the complexity to find solutions. An alternative approach for confined systems is the k.p method [2]. In the k.p formalism, the interactions among the different energy bands of a semiconductor are described by parameters in the matrix form of the hamiltonian. The construction of this matrix is generally made using group theory and symmetry concepts, the k.p method itself does not provide the parameter value of a given compound. Therefore, to use the k.p method in confined systems one must construct the matrix hamiltonian for the chosen energy bands and assign values for the parameters, in order to describe the desired semiconductor material. In this study, the main goal is to investigate a fitting method to obtain the k.p parameters, comparing the analytical coefficients of the secular equation to the numerical values obtained from a target band structure. The approach to obtain the target energy bands of bulk materials is the QUANTUM ESPRESSO [3], a free-software suite for "ab initio" electronic structure calculations. Also, the Maple software is used to handle the analytical forms of the secular equation coefficients. In this work we derive complete sets of wurtzite k.p coeficients using the proposed method and analyse their use in heterostructure calculations.

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Landé g-factor in AlGaAs/AlAs single and double quantum wells

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We report on the spin dynamics of a high mobility two-dimensional electron gas in a AlxGa1-xAs/AlAs double quantum well structure. For high electron density samples, the g- factor was measured using time-resolved Kerr rotation technique. The g-factor tuning capability was observed by changing the aluminum content x independently in each well. Experiments demonstrated an unusual spin dephasing time robustness for high excitation power. The effect of the interaction between wells was analyzed in samples with different tunneling barriers. Results were compared with experiments on single well systems demonstrating higher spin polarization generation, longer spin dephasing time, and coupling for the double structures.

Laser irradiations effects on the optical properties of PPV/synthetic dyes thin films converted at low temperatures

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The conjugated, light-emitting poly(p-phenylene vinylene) (PPV) is promising for use in optoelectronic applications, such as polymer light-emitting diodes (PLEDs) and photocells. This possible use is due to the significant progress in finding new routes to synthesize PPV from a soluble, non-conjugated polymer precursor, namely poly (xylylidenetetrahydrothiophenium chloride) (PTHT). PTHT films are converted into PPV films through a thermal treatment, for about 6 h, in which the tetrahydrothiophenium lateral group is eliminated, generally at high temperatures (higher than 200C°), under vacuum. However, the films resulting from this procedure have, generally, limited optical properties due to the formation of light suppressor defects, such as carbonyl groups. Recently, Marletta et. al. developed an alternative route to the chemical synthesis where the PPV can be obtained at a lower temperature by using the dodecylbenzenesulfonate (DBS) anion as counter-ion of the PTHT polymer. It was observed a significant improvement with the introduction of DBS, it being possible conversion to PPV at lower temperatures (100 °C) and time intervals considerably shorter ($\sim$ 30 min.) without compromising the optical properties of PPV. In the present work, the alternative route of conversion of PPV is adopted, however, rather than the DBS, three different synthetic dyes are used: Nitrazine Yellow (PPV/Nitrazine); Orange 2 Sodium Salt c (PPV/Orange) and Indigo Carmine (PPV/Indigo). A study of the laser irradiation effects on the optical properties of layer-by-layer PPV + dyes was carried out, where the samples were photo-irradiated with a polarized laser for about 60 min. The results show a strong increase in the PPV emission intensity with the photo-irradiation time for PPV/Nitrazine and PPV/Orange samples. This increase is not observed for PPV/Indigo sample. This result is attributed to the differences in the molecular structure of the dyes and, in particular, due to the fact that the Nitrazine and Orange have azo groups in their structure which allows the movement and alignment of azo chromophores through photoinduced isomerization cycles trans-cis-trans caused by excitation with polarised light. The PPV emission increase is attributed to changes in the conformation of the PPV chains caused by photo-irradiation combined with the energy transfer effect between the PPV and the segments containing the dyes and also a degradation of the dye molecules.

Linear Characterization of THz DFG Emitters

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Optical generation of THz via Difference Frequency Generation (DFG) provides an attractive technique for the fabrication of CW sources working at room temperature. Integrating the pump lasers and maximizing the nonlinear conversion efficiency are the biggest challenges related to such devices. In this context, a first approach based on DFG in dual-wavelength mid-IR quantum cascade lasers has been successfully exploited to demonstrate THz sources providing quasi-CW operation up to room temperature [1, 2]. We present in our contribution the optical characterization of an active THz source based on DFG between Whispering Gallery Modes (WGMs) sustained by triply resonant AlGaAs microcylinders, in which the active medium is provided by InAs Quantum Dots (QDs) embedded in the cavity central layer [3]. The simultaneous lasing of two near-IR WGMs is possible thanks to the inhomogeneous broadening of the QD gain profile and has been demonstrated at room temperature under electrical pumping [4]. These laser modes provide the pump fields for the DFG process, which is based on non-resonant $\chi(2)$ of bulk AlGaAs, with pump and DFG modes lying on opposite sides of the Restrahlen band.

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Linear Magnetoresistance on p-type PbTe samples

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The multiple applications of PbTe and its unique physical properties make it an attractive research subject. Its applications include solar cells, infrared sensors, thermoelectric devices and, recently, it was reported that it is also suitable for spintronic applications. Its dielectric constant (¿1400 at 4.2 K) leads to an effective screening against ionized impurities and defects which increases considerably the carriers mobility. In addition, the physics is further enriched by the large value of the Landé g factor and the small effective mass; both of which display considerable anisotropy.

The results that will be presented in this work show that the introduction of BaF2 in PbTe samples can convert the classical magnetoresistance, which is quadratic in magnetic field, in a large and linear function of the magnetic field that does not saturates even for B up to 17 T. In fact, a linear magnetoresistance has been predicted to manifest itself in semi-metals and narrow gap semi-conductors having tiny pockets of Fermi surface with small effective mass [Nature Materials, 7, 697 (2008)]. The results will be analyzed used the Parish-Littlewood model and the Quantum Magnetoresistance model developed by Abrikosov. In addition, the results suggest that the linear magnetoresistance can also be part of the transport that takes place at surface states due to the strong spin-orbit coupling intrinsic to narrow gap semiconductors. The results of the measurements will be also compared with results obtained for other IV-VI compounds like PbSnTe and PbEuTe. The final analyses performed on the experimental data will allow one to obtain a general pictures of the linear magnetoresistance effect on IV-VI materials.

Magnetic metastability of Sn0.96TM0.04O2, where TM = V, Cr, Mn, Fe, Co and Ni: an ab initio investigation

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Transition-metal (TM)-doped diluted magnetic oxides (DMOs) have attracted attention from both experimental and theoretical points of view due to their potential use in spintronics towards new nanostructured devices and new technologies. In the present work, we study the magnetic properties of Sn0.96TM0.04O2, where TM = V, Cr, Mn, Fe, Co and Ni. Spin-polarized electronic structure calculations were performed using the Projector-Augmented-Wave method as implemented in the Vienna Ab-initio Simulation Package, within density functional theory and the local density approximation. The calculated total energy as a function of the total magnetic moment per cell shows a magnetic metastability, corresponding to a ground state, respectively, with 1, 2, 3, 2, 1 and 0 μB/cell, for V, Cr, Mn, Fe, Co and Ni. Metastable states for Cr, Mn, Fe and Co were found. For V, Cr, Mn the ground state presents a high-spin configuration while it is allow low-spin configuration for Ni and Co. For Fe two high-spin configuration were found, with m = 2 and 4 μB/cell, where the first is the ground state one. The spin-crossover energies (ES) were calculated. The values are ESCr0/2 = 93 meV, ESMn1/3 = 42 meV, ESFe0/2 = 107 meV, ESFe4/2 = 25 meV, ESCo3/1 = 36 meV. Our results suggest that these materials may be used in devices for spintrônica applications that require different magnetization states.

Magnetotunneling through a THz coherent phonon generator

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In this work we study the resonant tunneling through a double barrier heterostructure (HDB) considering the electron-phonon interaction in the presence of a magnetic field parallel to the tunneling current. The system is described by a thight-binding Hamiltonian that includes the electrons, the phonons and the electron-phonon interaction.

$$H_{tot} = \sum_{j,l}(\epsilon_j + E_l - 2v)c^{\dagger}_{j,l}c_{j,l} + v(c^{\dagger}_{j,l}c_{j+1,l} + c^{\dagger}_{j+1,l}c_{j,l}) + \sum_{q}\hbar\omega_0 b^{\dagger}b + \sum_{q,l,l'}\frac{M_0}{\sqrt{V_0}q}\langle l'|e^{i\mathbf{q}\cdot\mathbf{r}}|l\rangle(b^{\dagger}_q + b_q)c^{\dagger}_{0,l'}c_{0,l}$$

The device is a heterostructure composed of GaAs/AlGaAs. This is controlled by an external potential. For a given bias electrons decay from the excited state in the well to the ground state by emitting primary optical phonons (LO_1). Such phonons decay into a secondary longitudinal optical phonon (LO_2) and a transverse acoustic phonon (TA). The phonons (TA) form a coherent beam in the terahertz range (THz), thus defining the Saser [**?**].

In order to calculate the transmittance and the electron current at finite temperatures, nonequilibrium Keldysh Green functions are used, We solve a system of kinetic equations that describes the dynamics of the electrons and phonons in the saser. The TA beam is useful because it corresponds to the lowest phonon branch. Therefore these phonons have a very long lifetime and a mean free path that could reach more than one centimeter. In the limit of low temperatures our results coincide with those obtained previously.

We consider several Landau levels that, besides the LO phonons, open new channels for the flow of electrons in the device. The results for resonant magnetotuneling are in agreement with experimental observations and other theoretical studies.

Many-Body effects on the Optical Properties of Quantum Wells Mn delta-doped Barriers

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Ferromagnetic semiconductors have attracted much attention in the last years not only for its potential of applications but also for its physics properties, e.g., spin-Seebeck effect in GaMnAs [1]. The incorporation of Mn ions on GaAs semiconductor still is a growth challenge, the transport and optical properties of the devices being affected by the presence of interstitial Mn. In order to obtain good transport and optical response of this ferromagnetic devices quantum wells (QWs) with Mn doping barriers have been investigated [2,3].

Recent magneto-optical measurements in InGaAs QWs with GaAs barriers with δ-doped layers of Mn and C show strong oscillations on circularly polarized QW emission as a function of the magnetic field. The emission of a right and left circularly light oscillates in opposite direction and their amplitude increases with the Mn content. The oscillations persist up to 25 K [2]. In order to understand these magneto-oscillations we studied the electronic and optical properties of the two-dimensional hole gas (2DHG) formed in the QW. The holes are provided by both Mn and C doping.

We used the spin-density functional theory within the $\mathbf{k}\cdot\mathbf{p}$ band description, the envelope function and the virtual crystal approximations to describe the electronic states of the system. The *sp-d* interaction was described by the Zener kinetic-exchange model. The Mnδ-doping was described by a two-Gaussian distribution that represents the Mn diffusion.

Our results show that when an external magnetic field is applied a 2DHG is formed in the carbon doped layer. This field affects the charge redistribution of the system inducing strong oscillations in both Fermi and energy levels, and consequently in the QW emission. The oscillations are caused by charge transfer between the QW and the gas in the carbon layer and also by the depopulation of the Landau Levels. We observed that exchange-correlation potential is responsible for the opposite oscillations observed in the right and left circularly emission, but the nature of this oscillations depend on the the nature of the Mn doping, in particular the distance between the QW and Mn layer, and Mn diffusion. This work is supported by FAPESP and CAPES.

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MD simulation of bulk and nanowire InP

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Using molecular dynamics (MD), we simulate structures properties of semiconductor InP. The interaction potentials used in our MD simulations consist of two- and three-body interaction terms. This potential provides excellent estimates for the vibrational density of states, melting temperature, structural phase transformation induced by pressure, and specific heat.The InP was described and compared in a bulk system and nanowires (NW) for different sizes and at various temperatures. The vibrational phonon density of states (VDOS) computed from MD calculations for a bulk system is in excellent agreement with the VDOS extracted from the rigid ion model (RIM), which is based on experimental results. The MD results reproduce very well the main characteristics of the experimental results, predicting the existence of the transversal optical and longitudinal optical modes, and a gaps. The effect of the surfaces on the VDOS of the NW is also shown. The main NW characteristics in the VDOS resemble the bulk results; however, some differences can be observed. The presence of the NW surface increases the density of modes in the gap region. The origin of the modes can be seeing through the partial VDOS for bulk and InP NW considering the In and P contribution separately. We notice that the P atoms make the main contribution to the optical modes, because such modes are characterized by the relative displacement between ions and lighter atoms usually dominate such dynamics. The effect of temperature on the VDOS for both NW and bulk structure is shown. We see a general broadening of the modes and a shift in the peak position to lower frequencies when the temperature is raised. Although the gap region keeps a similar profile, the VDOS increases with temperature. Moreover, the temperature affects the contrast between LO and TO modes, especially for the NW, where the LO frequency width increases. Notice that the mode broadening is slightly weaker for the NW than for the bulk.

Measuring Bipartite Quantum Correlations in NMR Systems

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How quantum states differ from classical states? For a long time, entanglement was considered the only responsible for that difference. When it was demonstrated that it is not possible to produce entanglement in conventional room temperature liquid state NMR, the use of the technique as a test bench for quantum information processing (QIP) was severely criticized. This last until it was shown that separable states, as found in most of the NMR implementations, may present other types of non-classical correlations, for instance, the quantum discord proposed by Ollivier and Zurek. Besides a time costly quantum state tomography process, the experimental evaluation of the quantum discord involves large number of mathematical manipulations. Because of that, other alternative discord measures have been proposed. For a two qubit system, Girolami and Adesso proposed the quantity Q(ρ), which allow the calculation of the so called geometric quantum discord DG, and Nakano et al. defined another discord measurement, named the negativity of quantumness QNA. We demonstrate that in NMR systems both quantifiers are calculated from spin correlations, which are measured directly from the magnetization of one nucleus (qubit) after applying a specific pulse sequence. The equivalency between direct and tomography based measurements of DG and QNA is then demonstrated using a two-qubit NMR system implemented by J-coupled 1H and 13C nuclei. Thereafter, we apply these quantities to determine the relative amount of quantum correlations present in two-qubit pseudo-pure states typically used in NMR QIP. At last, NMR is used to experimentally observe that, for some selected states and finite time period, the amount of discord is preserved even under the presence of relaxation (freezing of quantum correlations). We further observe the phenomenon of sudden change in the relaxation behavior of quantum correlations as measured by DG and QNA.

Keywords quantum information; quantum discord; geometric discord.

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Melanin Thin Films as Sensitive Membrane in Extended Gate Field Effect Transistors

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Nowadays the development of pH sensors is of great interest due to its extensive application in various areas such as industrial processes, biochemistry and particularly in medical diagnostics, measuring extracellular pH-related signals on cells and tissues. The extended-gate field-effect transistors (EGFETs) are devices able to detected the pH changes and are considered an alternative for the replacement of the conventional ion-sensitive field-effect transistor (ISFET) due its lower cost, simpler packaging and better long-term stability. EGFETs are constructed by an ion sensitive membrane connected to a commercial MOSFET. The search for membranes with higher sensitivities is the aim of several studies, in order to improve pH sensors development. There are many options of materials that could be used as ion sensitive membranes, as transition metals oxides. Besides these materials, the melanin, a class of natural pigments, is a promising conjugate polymer that due their structure has physical and electrical properties of great interest for application in biosensors. Furthermore, the use of organic materials in this type of device is interesting due to its low cost, ease purification and processing. In addition there is the possibility of deposition on a large variety of substrates, including flexible. In this work it was constructed an EGFET using melanin thin films as active membrane, attached to a commercial CD4007UB MOSFET. Melanin was synthesized by the oxidation of L-3-(3,4-dihydroxyphenyl)-alanine (L-Dopa) in aqueous medium. Thin films were deposited from a solution of melanin by spin coating technique on two different substrates (Indium tin oxide coated glass- ITO and gold coated glass - Au). The structure of the films were investigated by Atomic Force Microscopy and showed that the surfaces of the melanin films are very regular. Experiments were performed in order to obtain the response of the EGFET device when inserted into solutions with pH range from 2 to 12. The results showed that EGFETs with melanin deposited on ITO and on Au showed sensitivity of 44 mV/pH and 51 mV/pH respectively. Moreover both results are linear across all pH range studied. In conclusion, the use of melanin as an active membrane for use as biosensor EGFETs has shown to be promising due of their easy processing and high sensitivity.

Morphological Characterization of CdTe/Si(001) Thin Films

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Recently, CdTe/Si(001) films have attracted a lot of attention due to its potential as platform for the subsequent growth of HgCdTe, which is the most widely used material in infrared focal plane arrays and X-ray detectors of high performance. Several techniques such as MOCVD, MBE and HWE have been employed to achieve CdTe epitaxial layers on Si substrates of high crystalline quality. However, the large lattice mismatch (19% at 25 °C) and thermal expansion coefficient difference (46.9% at 25 °C) are relevant obstacles to growth process. Independently of production method, it has been shown that the grain size and surface morphology are some of the most important aspects affecting the properties of the films produced and the efficiency of the devices constructed. In this work, we have studied the interface and surface grains evolution of CdTe/Si(001) thin films by scaling dynamics theory (SDT), atomic force microscopy (AFM) and X-ray diffraction (XRD). The samples were produced by HWE technique, varying the substrate temperature from 150 to 300 °C and the films thickness from 0.2 to 3.2 μm. The results have shown that growth exponent decreases linearly with temperature increase from 0.45 to 0.18, while local roughness exponent changes, approximately, as power law with time, which is related to variations in aspect ration of grains due to coalescence process between neighbor grains. Moreover, this exponent approaches to 1.00 for high growth time and high temperature substrate, due to robust forms of grains, as corroborated by AFM and theoretically provided by Oliveira, T. J. et. al. (2011). The dynamic exponent, found through correlation function slope-slope, changes from 2.00 to 2.50 for temperatures between 200 and 300°C, while the kappa exponent (originated from dynamic evolutions of local inclinations) changes, linearly, with temperature from 0.33 to -0.57 for range from 150 to 300 °C. We also have found, an inverse anomalous scaling for the roughness, never reported to literature before, characterized by kappa negative values, which begins for temperatures bigger than 216°C. Finally, XRD measurements have shown that grains in (111) direction represents 60% of interface crystalline composition for thickness equals to 0.2 μm, and ¿96% for thickness bigger than 0.8 μm. It's evidenced that from this thickness, the film is highly textured.

Non-monotonic spin relaxation and decoherence in graphene quantum dots with spin-orbit interactions

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We investigate the spin relaxation and decoherence in a single-electron graphene quantum dot with Rashba and intrinsic spin-orbit interactions. The emergence of a nonmonotonic dependence of the spin relaxation time T_1 on the external magnetic field is attributed to the Rashba spin-orbit coupling-induced anticrossing of opposite spin states. A rapid decrease of T_1 occurs when the spin and orbital relaxation rates become comparable in the vicinity of the spin-mixing anticrossing. On the other hand, the intrinsic spin-orbit interaction leads to a monotonic magnetic field dependence of the spin relaxation rate which is caused solely by the direct spin-phonon coupling mechanism. The decoherence time is dominated by relaxation processes $T_2 = 2T_1$ for the electron-phonon coupling mechanisms in graphene up to leading order for spin-orbit interaction. Moreover, we show that the energy anticrossing also leads to a vanishing pure spin dephasing rate for these states for a super-Ohmic bath.

On the compositional issues in the preparation of Cu2ZnSnS4 films by spray pyrolysis technique under inert atmosphere

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Pneumatic spray pyrolysis thin films of Cu2ZnSnS4 (CZTS) were reproducibly deposited on soda lime glass and Mo-coated glass by using a special reactor designed for working under controlled atmosphere. The films were grown using Ar as the carrier gas under an Ar atmosphere. The variation of the concentration of CuCl2 and Zn(OOCCH3)2 used to prepare the starting-dissolution, as well as the post-thermal annealing treatment conditions on the compositional and physical properties of the films were studied. Annealing the films at 580 °C by 30 minutes highly improves its crystallinity and better assists the incorporation of Sn in the films. The optical band gap of the annealed films was found to be 1.48 – 1.50 eV. By Raman scattering the presence of ZnO compound was found to be present in the as grown films which we propose it becomes ZnS binary phase after annealing. Solar cells were fabricated using a Glass/Mo/CZTS/CdS/ZnO/ZnO:Al structure with the best results up to now of a good open- circuit voltage of 361 mV, a short-circuit current density of 7.5 mA/cm2, a fill factor of 37,1%, and an efficiency of 1.0%, with metallic ratios Cu/(Sn+Zn) Zn/Sn, Cu/Zn of 0.80, 1.17, 1.48, respectively. To our knowledge, this is the best efficiency value reported to date on a CZTS thin-film solar cell prepared by pneumatic spray pyrolysis, whose results are presented and discussed.

Optical phonon modes of wurtzite InP single nanowires

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Semiconductor nanostructures, in particular nanowires, have become a trend to engineer electronic and opto-electronic devices. In special, InP nanowires have attracted attention to the scientific community in the last years due to their intrinsic properties, such as low surface capture velocity and direct band-gap, which are technological important factors for optical device applications. Although its more stable crystal phase in bulk is zincblende, wurtzite phase has been reported for nanowires. The fact that these two phases, zincblende and wurtzite, have different unit cells and different symmetries, they result in different band structures [1] and phonon dispersion relations [2], which can affect directly the optical and thermal properties.

In this contribution we report on the investigation of optical vibration modes of InP nanowires in the wurtzite phase by Raman scattering spectroscopy. The nanowires were grown along the [0001] axis by the vapor-liquid-solid method using Au nanoparticles as catalyst in a chemical beam epitaxy system. The A1(TO), E2h and E1(TO) phonon modes of the wurtzite phase are identified by using linearly polarized light with different configurations relative to the single nanowire axes in backscattering configuration. Additionally, forbidden longitudinal optical modes have also been observed. By applying an extended 11-parameter rigid-ion model, using the same parameter given for the zincblende phase, the complete dispersion relations of InP in the wurtzite phase have been calculated, obtaining a good agreement with the Raman scattering results. In order to keep the same number of parameters the wurzite structure is assumed packed.

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Optical properties of a type-II quantum dot/quantum well hybrid structure

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In type II quantum dots only one of the carriers is confined in the dot, surrounded by the other carrier by Coulomb attraction that remains in the second material. The latter carrier is usually weakly bound and can thus be easily ionized by, for example, increasing temperatures. This can be a limitation for certain device applications. Using a quantum well nearby the dots is an alternative to localize both carriers maintaining the desired properties of the structure. Hybrid structures involving quantum dots and quantum wells have been frequently used for optical devices based on type-I systems for various purposes, including a way to provide a rapid carrier transference of carriers to the dots. For type-II systems, where electrons and holes can be spatially separated in distinct regions, the hybrid structure provides an extra degree of freedom that may be used to control the optical transitions. In this work, we investigated the optical properties of GaSb/AlGaAs quantum dots coupled to a GaAs/ AlGaAs quantum well. The optical transitions of this hybrid structure are in the near infra-red range, which is adequate for optical device applications. We analyzed samples with different separations between the GaAs/AlGaAs quantum well and the GaSb/AlGaAs quantum dots. For large spacer layer samples, we only observed optical transitions associated to the quantum well. The main emission band is accompanied by a lower-energy shoulder. Both bands present short decay times (300 ps), which corroborates their attribution to type-I quantum well recombination. We propose that the low energy shoulder is due to localized states induced by the strain field created by the GaSb dots. For smaller spacer layer samples, the quantum well emissions become weaker and two additional lower-energy broad emission bands arise. The broad bands present long decay times (tens of ns), and they are therefore attributed to spatially-indirect transitions involving an electron localized in the GaAs quantum well and a hole in the GaSb wetting layer and GaSb quantum dots, respectively. Photoluminescence excitation results also reveal the coupling effect in the hybrid structure. The quantum well-quantum dots hybrid structure is therefore a promise system for optical applications.

Optical properties of high quality GaAs/GaAsP core-shell nanowires on silicon

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Incorporating light-emitting components into Si microelectronics has been the impetus behind the development of Si photonics for the last twenty years. The difficulty of such implementation lies on the lattice mismatch between Si and III-V semiconductors commonly used for generation of light. Semiconductor nanowires (NWs) have emerged as promising candidates for such III-V on Si integration since they present highly versatile nanostructures less reliant on the lattice-matching with the substrate than bulk semiconductors. In this contribution, we investigate the optical and structural properties of catalyst-free GaAs/GaAsP core-shell nanowires (NWs) grown on Si(111) substrates using molecular beam epitaxy. Using micro-photoluminescence (micro-PL) spectroscopy, we investigate the emission properties of single GaAs/GaAsP NWs and compare them with similar GaAs NWs which have the surface exposed to air. We find that GaAsP capping leads to strained core-shell structures with strong PL emission at energies above zinc-blende GaAs band-gap. Using time-resolved micro-PL we find carrier lifetimes between 1 and 2 ns at low temperature and PL linewidths of the order of 20-50 meV. Uncapped GaAs NWs exhibit a wide range of carrier lifetimes from 0.3 up to 7.4 ns spanned along an energy range of approximately 120 meV below the GaAs bandgap at 1.515 eV. Such distribution of carrier lifetimes is consistent with type-I and type-II electron-hole alignment along the axis of single NWs containing both zinc-blende and wurtzite GaAs crystal structures. We also investigate the effects of GaAsP capping on the surface states and oxidation of single NWs. We demonstrate that in core-shell structures PL is strongly enhanced as compared to uncapped GaAs NWs due to efficient surface passivation. At 77 K, an enhancement factor of 3x104 is obtained, which leads to easy PL detection at room temperature for GaAs/GaAsP structures. In contrast, PL emission in uncapped NWs is strongly quenched for temperatures above 60 K as a result of non-radiative recombination paths associated with the high density of surface states. Mircor-PL temperature dependence measurements in the core-shell structures enable the determination of activation energies. At higher temperatures, we demonstrate that the main PL quenching mechanism in core-shell single NWs is associated with the escape of holes from the GaAs core to the GaAsP shell.

Optical properties of Mn-implanted quantum wells

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Spintronics seeks for new materials that are suitable for controlling the spin degree of freedom for information transport and processing. One of the approaches devised to manipulate the carriers' spin is the addition of magnetic ions such as Manganese in conventional semiconductor materials. Efforts in this direction lead mostly to growth of diluted magnetic semiconductors such as MnAs or GaMnAs. In the present work we investigate an alternative path by reporting on the effects of Mn ion implantation on the optical properties of semiconductor quaternary quantum wells (QW) in order to assess its potential for spintronics. The samples consist of 40 nm InGaAsP quaternary QWs grown by metal-organic chemical vapor deposition on GaAs (001) substrates. Barriers and well alloy compositions were adjusted so that the QW emission lies close to 1.5 m. Mn ions were implanted at different doses (1, 10 and 20 at.%) and annealed at two temperatures (650 oC or 750 oC). We also kept a set of as-implanted samples, as well as the as-grown QW for comparison purposes. Low-temperature photoluminecence (PL) measurements revealed that even after thermal treatment some of the samples did not recover from the usual damages induced by the ion implantation process. Samples treated at 650 oC showed good recovery of substrate light emission efficiency, however the QW signal is not present, except for the sample with 20 at.% Mn implantation. The 750 oC treatment led to better results since there is a presence of an emission band around 1050 nm. The best recover was found, again, for samples with 20 at.% Mn, which seemed unusual since one expects that a higher implantation dosis would lead to an increased number of induced defects, thus the recovering of a good optical emission signal should be more difficult than for other Mn dosis. In our case the sample with highest Mn contents present the better PL spectrum. However the strong energy blue shift of PL peak, when compared to the non-implanted sample emission spectrum, might be related to a softening of quantum well interface due to thermal annealing. Also the PL efficiency of non-implanted QW samples seems to play an additional role.

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Optical properties of oxide glasses with semiconductor nanoparticles co-doped with rare earths ions

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The aim of this work is to determine the influence of semiconductor nanoparticles in the optical emission of rare earth ions in glassy matrices. The two systems studied are: (a) PZABP + [1Te + 2Yb2O + xEu2O3] (wt %), and (b) PZABP + [2Yb2O + xEu2O3] (wt %), where x = 1;2;3;4;5. The former systems are PZABP glassy matrices with nominal composition [60P2O5 .15ZnO . 5Al2O3 . 10BaO . 10PbO] (mol %) doped with ZnTe nanoparticles and co-doped with rare earth ions, Ytterbium (Yb3+) and different concentrations of Europium (Eu3+). The latter samples are the references ones co-doped with rare earths ions Yb3+ and Eu3+ without Te. Optical absorption, photoluminescence and time-resolved photoluminescence techniques have been used to characterize the samples in order to investigate the possible energy transfer mechanisms that may occur due to the various compositions of the samples. Radiative lifetimes have been obtained by means of Judd-Ofelt theory and also through experimental measurements with the purpose of calculating quantum efficiencies of the samples. From our results we have verified the influence of the nanoparticles in the optical properties of Ytterbium ions. Energy transfer between the ZnTe and Yb3+ may occur as an increase in the emission intensity of the Yb3+ was observed when the nanoparticles were present. Such results may be important for applications in high power lasers, optical amplifiers, ultra short pulses lasers and tunable lasers in the infrared region from 920 nm to 1060nm. We would like to thank the Brazilian Agencies: CNPq, CAPES, FAPEMIG, FAPEAM, IFAM and UFJF.

Optical studies of a 2DEG in double quantum wells

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The influence of a dense two-dimensional gas in the trion and exciton optical transitions of a single quantum well has been extensively studied. Adding an extra control parameter, bilayer systems can be constructed by two parallel quantum wells with a high mobility electron gas separated by the tunneling barrier. When a magnetic field is applied perpendicular to well plane, the quantum Hall states are formed. For double wells with vanishing g-factor, experiments reveal unsual magneto-transport features in the quantum Hall effect. The possibility to generate direct and indirect excitonic states in double quantum wells focused great attention in optical experiments. Here we study AlGaAs/AlAs single and double quantum wells by independently adjusting the Al content in a pair of square quantum wells with equal width.

Optical transitions on III-V heterostructures subjected to external electric field

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Semiconductor heterostructures have been studied since the last decades due to their important electrical and optical properties such as the ability to emit light at a specific wavelength with high efficiency. In the present work we present experimental measurements and numerical calculations referred to the study of the effect of external electric fields aligned along the growth direction of AlGaAsP quantum wells on the optical transition. The transition energy shift allows us to tune the emission energy and the absorption threshold, attributing technological applications such as the construction of an electro-optical device with tunable transmission band. We simulated various heterostructures to find the most sensitive to the application of the electric field and also analyzed the overlap integral between the electron and the hole wavefunctions in order to estimate the degree of oscillator strength of the recombination process. With the electric field ranging between zero and 50 kV/cm, type I square quantum wells (SQW) presented a transition energy shift below 1 meV, proving to be an inadequate structure for the intended purposes. Type II SQW showed a shift larger than 100 meV, however the overlap integral vanishes completely even for low applied electric fields. We also studied type I double parabolic quantum wells (DPQW) and a type II heterostructure with lattice matched AlGaAsP alloys. The energy shift for the DPQW was about 44 meV, and for the type II structure was slightly larger, 48 meV. Both cases had no significant decrease in the overlap integral. The results suggest that these two latter structures present potential application in contrast to the conventional SQWs.

OXIDATION OF InP NANOWIRES: A FIRST PRINCIPLES STUDY

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A study of InP nanowires with an oxide layer, as well as the initial steps of the oxidation process is pursued through first principles calculations and molecular dynamics simulations within the Density Functional Theory. An InP nanowire in the wurtzite phase in an environment containing a O2 molecular gas is used to simulate the initial steps of the nanowire oxidation process. The molecular dynamics simulations reveal that the O2 molecules dissociate preferentially in reactions with the P atoms and that that they are incorporated into the nanowire, mainly at the superficial layers. The molecular dynamics simulation of the already oxidated InP nanowire reveals a pair distribution function very close to that of the pure nanowire, although there is a disarrangement of the local crystalline phase. The defects generated by the atoms lead to the closure of the energy gap, due mainly to the contribuition coming rom the In atoms bond to oxygen.

Phonon Localization in cubic GaN/AlN superlattices

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Wide-bandgap heterostructures based on group-III nitrides present a great interest due to the applications in optoelectronic devices. Usually, the development of these devices employs the hexagonal phase of GaN which has the disadvantage to produce built-in electric fields. This is a factor that limits the performance of optoelectronic due the induced quantum-confined Stark Effect. However, the high crystal symmetry of metastable cubic phase of GaN and AlN presents no polarization field in (001) growth direction. Many efforts have been done to develop high crystal quality nitrides, reducing the surface roughness of layers and optimizing the hetero-interface and structural quality of multilayer stacks. To enhance the devices performance a better understanding about the confinement of polar optical-phonons in the heterostructures should be achieved. In this work, we investigated a serie of three GaN/AlN superlattices (SL) grown by plasma-assisted Molecular Beam Epitaxy (MBE) on 3C-SiC substrates. The samples consist of 100 periods of 3nm AlN barrier with well thicknesses: L1= 4nm, L2= 7nm and L3= 10nm. The optimal stoichiometry conditions for the epitaxial growth and the thickness of layers were monitored by in-situ reflection high energy electron diffraction (RHEED). Reciprocal Space Mapping (RSM) measured by high resolution X-ray diffraction (HRXRD) at the (113) reflections reveals the SL satellites peaks and the strain in the structures. Photoluminescence (PL) spectra show the emission due to the confined states of SL. Raman spectra at room temperature were recorded by a triple grating spectrometer, with microscope facilities, using line 568.2nm of an Ar+/Kr+ laser as excitation source. The bands attributed to TO phonons, activated by disorder, were identified at 560cm-1 due to GaN and 635cm-1 to the TO phonons in AlN, red shifted due to the strain. The GaN LO phonons at 741cm-1 have an asymmetric shape attributed to the density of states influence due to the finite coherence length (Lc), which allows excitations with q ¿ 0 to contribute to the Raman intensity. An optical phonon confinement model is used for calculating the theoretical line shapes, which exhibit different asymmetric broadening and shifts, depending on the symmetries of phonon and their dispersion curves. The Lc of LO phonons in the GaN determined by these analyses are in good agreement with the thicknesses of the layers in which they must be localized.

Photocurrent control by dynamic localization effects in a multiple quantum well structure

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The photocurrent spectra of a multiple quantum well heterostructure (MQW) under electric field varying since zero to Stark-strong fields is exactly calculated by using a split-operator numerical approach, which also yields full knowledge of MQW eigen-states and eigen-energies. The idealized structure is made of ten 5 nm GaAs quantum wells spaced by 11 nm AlGaAs barriers. Narrower AlGaAs filter barriers, whose heights roughly coincide with the depth of the wells, are placed on top and at the center of each spacing barrier to provide a filtering effect that leads to the formation of a quasi-discrete set of states in the continuum. Under the application of both static and dynamic (photon) electric fields, the calculated photocurrent shows effects of the Wannier-Stark localization in the shifting of some of its peaks. For low biases the photocurrent shows both negative (owing opposite to the expected direction) and positive peaks at different incident-photon frequencies. As the bias increases, only positive photocurrents are generated at all frequencies, and the overall intensity of the main peak reaches a minimum value before presenting peaks with the bias. These results are understood in terms of the dynamic localization effects due to the avoided crossings between localized and extended states belonging to specific parts of the heterostructure.

Photoluminescence studies of Mn-containing InAs quantum dots grown by molecular beam epitaxy

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Recently, considerable efforts have been made to investigate quantum dots (QDs). In the strong confinement regime, QDs are special in their δ-like density of states, strong ability to capture carriers and high photon emission efficiency because of the quantum confinement in three dimensions. Incorporating magnetic atoms into semiconductors to fabricate diluted magnetic semiconductors (DMS) can create a local magnetic field and result in giant Zeeman splitting for the sp–d exchange interaction between the band carriers and the magnetic atoms. Therefore, DMS materials have attracted much attention for both the investigation of fundamental physics and their promising applications in spintronic devices. Among DMS structures, InMnAs quantum structures have become particularly attractive because they combine the properties of InAs QDs and Mn ferromagnetic compounds. The hybridization between the quantum-confined holes in the QDs and the itinerant holes in the semiconductor valence band makes it possible for holes to transfer between the DMS QDs, which can induce the long-range ferromagnetic order of the localized spins. It is difficult to introduce Mn atoms into III–V-based self-assembled QDs because of the low solubility. Several special growth methods have been investigated to fabricate InMnAs QDs, such as low-temperature molecular beam epitaxy (LT-MBE). Driven by the above mentioned facts, InMnAs QDs grown on GaAs(100) substrates with different Mn concentrations were studied. The samples were grown using a RIBER 32P solid-source MBE apparatus. The InMnAs QDs were obtained by usual strained epitaxy, Stranski-Krastanov growth mode. The evolution of all process of the dots formation was monitored in-situ by Reflection High-Energy Electron Diffraction. The Manganese concentration was first determined by the In/Mn flux rate and confirmed a posteriori by the X-ray Grazing Incidence Diffraction scattering measurements, staying in the range of 0–1.6x10^{2}0cm$^-$3. The growth was realized at 320 ^{circ}C. In this work, we report a study of the photoluminescence (PL) characteristics of the referred samples. The PL measurements were performed in a variable-temperature (10–300K) closed-cycle cryostat under the excitation of the 514.5nm line of an argon laser, with power varying between 0.1–150mW. The luminescence was detected by a cooled InGaAs photodetector. The influence of Mn concentration, and the temperature and laser power dependence on the PL signal will be presented.

Polarization dependent photocurrent of InAs/AlGaAs quantum dot intermediate-band solar cells

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A semiconductor intermediate-band (IB) solar cell is an n-p photovoltaic device containing an active region which introduces energy levels between the conduction band (CB) and valence band of the hosting semiconductor.[1] The intention is that the IB levels will better distribute the optical transitions over the solar spectrum, in a similar way as the triple-junction solar cells do. Quantum dots can be used to create the IB levels, allowing some degree of adjustment of the levels due to the fact that the energy of the bound states in the dot can be controlled in the growth process through the dot dimensions and composition. Ideally, to take advantage of the full solar spectrum one needs transitions around three average energies: Eg = 1,93 eV, Em = 1,23 eV e El = 0,7 eV. While the higher energy transitions can occur exciting across the semiconductor gap (interband transitions), the lower energy transition involves intraband transitions promoting an electron in a dot-bound CB state to the unbound CB states (continuum). In this work we theoretically investigate an IB solar cell of InAs/AlGaAs quantum dots. These dots can provide levels allowing for the aforementioned energy transitions. We focus our investigation on the intraband transition studying the relative efficiency in generating photocurrent by different polarizations of the exciting radiation. The intraband transition is sensitive to the radiation polarization through the selection rules of the dipole transition. We have calculated the photocurrent for a cylindrical quantum dot due to the excitation of an electron in its ground state to the CB continuum. For that, we solved the effective-mass Schrödinger equation for the electron in the dot being excited by a time-dependent ac field acting as the infrared (IR) radiation with energy 0.7 eV. The dot level structure and the absorption coefficient are also calculated to clarify the transitions involved in the photocurrent generation. The polarization of the IR field is set either parallel or perpendicular to the dot plane to investigate the advantages in exploring both polarizations in an actual solar cell. The parallel polarization commonly occurs in normally incident light, but the perpendicular polarization can also be activated, for instance, by the use of a diffracting grating, therefore improving the cell efficiency with this additional excitation channel.

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Polaron Gas in GaAs Parabolic Quantum Well Wires

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The quasi-one-dimensional (Q1D) electron gas confined in semiconductor quantum well wires (QWW) has motivated a great number of experimental and theoretical studies, due to the potential application of the QWW in the electronic devices fabrication. The Q1D polaron gas present in these structures, composed of polar semiconductors, results from the coupling between the plasmons with the LO phonon field and has been investigated theoretically by several authors in the last few years. Particularly for rectangular GaAs QWW, results of many body theoretical calculation has reported observation of deeps in the static structure factor dispersion relation curves and the authors shown that such deeps are directly related with the resonant split of the intrasubband plasmon-LO phonon collective excitations energy. In this work we investigate the plasmon -LO-phonon interaction effects on the intrasubband static structure factor, pair correlation function, and the plasmon energy associated with the lowest subband in GaAs-AlGaAs parabolic QWW as a function of the electronic densities for several height of the potential barrier. Our calculations are performed using the Random Phase Approximation (RPA) at zero temperature. We show that the polaronic effect on the structure factor and on the pair-correlation function are more significant for lower electronic densities, just in the region where the RPA approach presents non-physical negative values for the pair correlation function. Therefore we also calculated the critical density from which this calculation method gives non-negative values for the pair-correlation function for small interparticle separation with and without the inclusion of the electron -LO phonon coupling. We found that for electronic densities greater than 4.1$\times$105 cm-1, the RPA may be used. This value is 17% higher than that computed previously in the literature.

Probing quantum dot-cavity coupling using a nearby empty cavity

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The future of solid-state quantum information processing is dependent on the possibility to coherently couple several qubits and let them interact. This implies in know all sources of decoherence and elaborate ways to avoid them in a state of a single qubit. For spins in quantum dots, which can be optically manipulated, a frequently discussed possibility is to use a common cavity mode for mediating interactions [1].

Recently A. Laucht *et al.* [2] presented a detailed theoretical and experimental investigations of electrically tunable single quantum dot (QD) - photonic crystal (PhC) nanocavity systems operating in the strong coupling regime of the light-matter interaction. They employ the quantum confined Stark-effect to electrically control the exciton-cavity detuning. Using this device they were able to systematically probe the emission spectrum of the strongly coupled system as a function of external control parameters, as for example the incoherent excitation power density or the lattice temperature. In another study [3], using a similar device, they investigate the coupling between two different QDs with a single cavity mode.

Here we developed a theory to investigate the emission spectrum of QD-PhC cavity coupled to another empty cavity. We study the requirements for analyze the QD-PhC cavity strong coupling looking at emission spectrum of empty cavity. We explore a wide range of parameters, as for example, the exciton-cavities detunings, (assuming that the QDs can be individually controlled by a local electric field), the excitation power of each QD, the spontaneous decay, and pure dephasing. We use density matrix formalism in the Lindblad form, and we solve it numerically. This can give new insights for future experimental measurement focusing on quantum information processing.

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Quantum dot optimization for Intermediate Band Solar Cells

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Intermediate Band Solar Cells (IBSC) is a new concept of semiconductor device capable of absorbing the solar radiation generating electrical power with high conversion efficiency. Ordinary solar cells have a single bandgap structure capable of absorbing a small section of the solar spectrum. A better approach is to use a tandem cell system with three coupled pn junctions, each one with optimized absorption for a different section of the spectrum; such structures have reached an efficiency of around 44%. Like the tandem structures, IBSCs are also capable of absorbing three different sections of the solar spectrum but having a single pn junction instead of three. An intermediate energy level within the IBSC structure bandgap makes this possible. There are several alternatives to introduce the intermediate band. One of them relies on the confinement of electrons inside a quantum dot (QD) system. Our calculations have shown that the efficiency of such solar cells can be optimized for the InAs/ GaAlAs system, where InAs QDs are nucleated on GaAlAs. A high density and uniform size distribution of QDs are imperative in order to reach the expected efficiency. Therefore a systematic investigation has been conducted on the nucleation of InAs QD on GaAlAs and the results shall be reported. In this work several InAs/GaAlAs quantum dot structures were grown by Metal Organic Vapour Phase Epitaxy (MOVPE) under different conditions. Growth temperature, growth rate, III/V ratio, annealing time and deposited material were varied and the produced quantum dot layers analyzed by atomic force and transmission electron microscopies, photoluminescence and reflectance anisotropy spectroscopy. The best compromise between density (1.7x1010QD/cm2) and homogeneity is achieved for a III/V ratio equal to 6.4, growth rate of 0.47ML/s, nominal thickness of 1.12ML, grown at 490 °C, with the annealing time set to 12s.

Quantum transport for holes through Q2D nitride-based multilayered superlattices.

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We develop a general approach to study multichannel-multiband transport properties through nitride-based multilayered systems. The theoretical model presented, take advantages of the analytical scheme to test the valence band spectrum of type-p doped semiconductors alloys[1] and transfer-scattering matrix technique within the multicomponent scattering approach (MSA)[2]. Apart with standard procedures, we deal simultaneously with all the accessible physical channels, then we are able to distinguish and to calculate transmission amplitudes, for each pair of incoming and outgoing traveling modes. Worthwhile to stress, that the conception of tunneling channel as well as the propagating modes representation became a major challenge, demanding from us a refinement of the theoretical treatment to avoid the intrinsic difficulties of the self-consistent calculation for hole levels. The last requires finite boundary conditions, yielding to discrete hole states. Importantly, the direct consequence for having confined out the hole states is the incompatibility with the MSA framework, due the propagating modes representation assumes incoming/outgoing fluxes to be unbounded at the source/drain electrodes. We manage this drawback by redefining the envisioned transport channels and selecting the scattering *cell* properly. The accurate inclusion of several cumbersome effects to setup the scatter-potential configuration, guarantees a more realistic description for quantum transport through nitride-compounded superlattices. As far as we know, earlier reports concerning the hole tunneling, disregard many of the truly involved potentials for nitrides. Thus our proposition for the effective potential, is yet another striking contribution of the present model to the quantum transport theory for holes, and suggest the possibility of forthcoming experimental measures for its confirmation.

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Quantum-cascade photodetectors for mid-infrared operation

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Traditional heterostructures used for mid-infrared photodetection, generally based on quantum wells (QWIPs) and quantum dots (QDIPs), suffer from intrinsic limitations in performance due to their high dark current and its associated noise, or to their low quantum efficiency. A few years ago, a quantum extractor, similar to the structure used in a quantum-cascade laser (QCL), was proposed as an elegant solution in order to lower the dark current and noise in QWIPs [1]. This new class of devices, called quantum-cascade detectors (QCDs), has great potential for mid-infrared photodetection. Indeed, since they operate at zero bias, most thermally excited carriers do not take part to the total current, thus reducing drastically the dark current. In addition, such devices are even more selective than ordinary QWIPs as they involve only transitions between confined states of the doped quantum wells that are used to absorb the incident infrared radiation.

In the present work, we developed a computational tool able to simulate the energy levels and wavefunction of such QCDs, using quantum dynamics [2]. The electron-phonon interaction was also included in the calculations in order to provide the total resistance of the device as a function of temperature. A QCD operating around 8 μm was successfully grown using moleculear beam epitaxy (MBE), processed by photolitography and fully tested. A blackbody responsivity of 90 mA/W and detectivity of 2.5×10^9 Jones were obtained at 80K. The width of the absorption spectrum (full width at half maximum) was only 0.8um. Further theoretical and experimental results will be addressed.

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Quasi-bond states in axial gated Graphene devices

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Graphene has attracted considerable attention due to its remarkable electronic and transport properties with promising technological applications in designing new nanoelectronic devices. Most of its intriguing spin and electronic properties arise as a consequence of the zero energy gap between the valence and conduction bands and the linearity of the low-lying energy dispersion relation. Thus the physical behavior of massless Fermions in graphene is described by Dirac equation instead of Schrödinger equation. The search for bound states in a usual non-relativistic quantum mechanics is a well known task, but it becomes a challenge for the Dirac equation due to the quasi-bound states and chirality which leads to several coupled equations to be solved simultaneously. In this work we propose different axial electrostatic confinements to engineer quasi-bond states by controlling gates voltages. After having showed, in a previous work [1] the influence of the voltage gate barrier on the quasi-bound states of the graphene-quantum ring (QR) emerged from a combined effect of the electrostatic confinement and the substrate-graphene interaction, we are able, in a natural extension, by exploding the cylindrical symmetry of the system, to manage different geometry profiles in order to assessing and tailoring these pseudo-relativistic bound states in nanostructures axially coupled. By only adding concentric front gates on the previous setup system [1], our new device conforms a radial potential profile which consists in a sequence of, an attractive core, a repulsive barrier and an attractive rim gates. In this new panorama, we study the interaction between the two nanostructures which give rise to new energy states due to new coupling degree of freedom. Although continue depending on the barrier width as usual, the spectra as function of this parameter has a peculiar behavior in contrast of the non-relativistic quantum systems. By fixing the quantum dot voltage and varying the others two (barrier and rim voltages) we have also new different pseudo-relativistic states defined by our phase diagram that became a useful tool to track the conditions under which these Dirac- confined states appear.

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QWIP's performance as a function of the quantum well doping

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Thanks to their homogeneity and material hardness Quantum Well Infrared Photodetectors (QWIPs) based on III-V semiconductors are already being used in focal plane arrays substituting the traditional so-called MCTs (based on alloys of HgCdTe). Even though already in the market, there is still much room for improvements in their performance. Important figures of merit of the detectors such as dark current, noise, responsivity and detectivity are influenced by various material parameters . In particular, we report that the doping level in the quantum wells of the devices affects the device performance differently depending on the figure of merit to be optimized. We have systematically investigated QWIPs based on InGaAs/InAlAS quantum wells grown by metalorganic vapor phase epitaxy lattice matched to the InP substrates as a function of the doping level. The three samples, A, B and C were n-doped to 6x10^{1}7cm-3, 2x10^{1}8cm-3 and 4x10^{1}8cm-3, respectively. Fifty periods of the 3 nm quantum wells and 30 nm barriers were grown between n-contact layers. X-ray diffraction and photoluminescence confirmed the composition and thickness of the different layers. Photocurrent measurements using a Fourier Transform spectrometer revealed that all samples show a peak around 4.1 m, as expected. Dark current measurements showed that, at low temperatures, the sample with intermediate doping level, B, presents a higher value. Sample C shows a lower dark current because the mobility decreases due to the increase in scattering, reducing the carriers drift velocity. And, at high temperatures ($\sim$150K), the thermally excited carriers density, which is related to the doping level, dictates the dark current behavior. At this temperature sample C has higher dark current than sample B. For sample A, the dark current is always limited by the thermally excited carrier density, since the doping density is too low. As expected, the responsivity measurements showed the same behavior as the dark current, meaning sample B has the highest value. Noise measurements were performed to determine the devices' detectivity and their results for the dark current could not be explained solely by the shot noise model, implying that there are different noise sources acting on the structures. As the noise is lowest for sample C, its detectivity showed the best value (2x1010cm.Hz1/2W-1). Therefore the sample with the higher quantum well doping density is the one that maximizes the detectivity.

Rashba effect in n-type PbTe/Pb1-xEuxTe Quantum Wells

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The Rashba effect is one of the manifestations of the spin-orbit coupling for electrons in semiconductors nanostructures and has been considered as one of the basis for new spintronic devices. One of the main issues remains in the determination of the factors and limitations that determine the strength of this coupling in different systems. Particularly, we are interested in the analysis of such phenomenon in structures made of PbTe, which is a IV-VI narrow direct gap semiconductor with small effective masses. Due the large Landé g factor of PbTe, the quantized conductance observed in nano structures exhibit a well-defined spin-splitting of the plateaus for low magnetic fields (lower than 1 T). This allows the development of spin-filters based on this material.

In this work, we have investigated the low-field magnetotransport properties of 10 nm and 14.5 nm n-type PbTe/ Pb1-xEuxTe quantum wells grown by molecular beam epitaxy on [111] oriented BaF2 substrates. The PbTe layers are surrounded by two 30 nm Pb1-xEuxTe (x = 0.13) barriers doped with Bi. Weak antilocalization has been observed in the magnetoresistance measurements as a function of temperature indicating the presence of the spin-orbit coupling effect. This confirms the theoretical predictions of the existence of strong Rashba effect for IV-VI lead salts (PbTe, PbSe and PbS) asymmetric quantum wells. Once PbTe has inversion symmetry we expect a negligible Dresselhaus spin-orbit splitting. As a consequence, PbTe quantum wells should present a spin-orbit splitting which is purely of Rashba type. Using the appropriate theoretical model we will calculate the spin-orbit and inelastic scattering times as functions of the temperature and carrier concentration for both quantum wells by means of the fitting performed on the experimental curves. Through this detailed analisis, we expect to shed some light on the Rashba effect on IV-VI quantum wells.

Refilling dynamics of compressive overlayers near an incommensurate structural transition.

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We investigate the time evolution of a coverage step profile in a compressively strained incommensurate overlayer, as a model for for the refilling dynamics of Pb wetting layers on the Si(111) surface [1, 2]. An extension of the two dimensional model introduced recently [3], displaying incommensurate striped and hexagonal phases of domain walls, is used to study the behavior near the striped to hexagonal structure phase transition. The results, obtained by Brownian nolecular dynamics simulation, shows the nucleation and growth of a domain of the hexagonal phase around the initial step profile in the striped phase. The behavior is qualitatively similar to those observed in recent experiments on the refilling dynamics of desorbed circular regions for the Pb/Si(111) interface [2].

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Resonant behaviour of phonons in a double barrier heterostructure

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The saser studied in this work consists of a coherent beam of transverse acoustic phonons (TA) of ultra-high-frequency which arise from the decay of longitudinal optical phonons LO_0 in $GaAs$. In a saser, longitudinal optical phonons LO_0 are created when electrons injected in the first excited level of a double barrier heterostructure system, decay to the ground state. The tuning of this device depends of an applied external potential so that the difference between the first excited level and the ground level stay near the LO_0 phonon energy, i.e., $E_1 - E_0 \approx \hbar\omega$, where ω is the frequency of longitudinal optical phonons LO_0 of $GaAs$ in the gamma point of the Brillouin zone. Phonons LO_0 decay in secondary longitudinal optical phonons LO_1 as well as in a beam of transverse acoustic phonons TA which are coherent. This coherent phonon beam is called saser. the phonons of the saser beam are emitted in the direction $[111]$ near the L point of the Brillouin zone. The (TA) phonons will accomplish multiple reflections in the double barrier, generating an accumulation of TA phonons in the well with wave vector parallel to interfaces. For a given U_{th} potential, the system organize itself, such that the other emission processes are enslaved. In other words, they are obliged to emit in the selected mode of the resonant cavity. As a result, we obtain a well-defined coherent (TA) phonon beam. In this work, we make a complete study of the resonant behavior of the TA phonons. We are interested in estimating the lifetime of phonons in the well. For this reason, we will develop, first of all, a mathematical method of a linear chain $1D$ with a single atom and with two atoms with and without translation symmetry simulating the interfaces. To the system without translation symmetry we define a transfer matrix among sites. We calculate the transmitance and the reflectance. Then we generalize the model to $3D$. First in a simple cubic lattice. Later in the zincblend lattice. By calculating the transmitance, we obtain the resonant peaks. From the width of resonant peaks, we estimate phonons lifetime in the double barrier heterostructure.

Search for Ferromagnetism due to Oxygen Vacancies in Co-doped SnO2

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Dilute magnetic semiconductors (DMS) have been intensively investigated since the publication of a theoretical work of Dietl [1]. With the exception of GaAs and CdTe, which present magnetic ordering at low temperatures when doped with Mn, no other materials were undoubtedly recognized to this application so far. However, many works have reported ferromagnetism at room temperature on (TM)-doped SnO2 samples, (TM = transition metals) [2]. First-principle calculations works have also reported ferromagnetism with the induced magnetic moment at TM atoms near oxygen vacancies [3]. Despite that, the origin of the ferromagnetism in TM is unclear and the confirmation of application of doped SnO2 as DMS is not established yet. In this work we have studied Co-doped SnO2 from an atomic point of view by measuring hyperfine interactions with perturbed gamma-gamma angular correlation spectroscopy (PAC). The films have a thickness of 100 nm which were deposited by sputtering on the Si (100) substrate. The films with 3% of Co were doped by ion implantion at 80 keV using the ion implanter Bonn Isotope Separator (BONIS), at the University of Bonn, the same machine that subsequently implanted the probe nuclei 111In with energy of 160 keV. The hyperfine parameters were studied as function of temperature and the measurements at room temperature were carry out with and without a magnetic field applied of 2.1 T. We compare these results with our previous work [4] where powder samples were measured. Ion implantation of the probe nuclei 111In was followed by a PAC measurement and subsequently by a thermal annealing at 873 K in vacuum. PAC results show the presence of two fraction sites for probe nuclei, one is the substitutional Sn site which corresponds to the rutile phase of SnO2, and the other was assigned to defect sites. We investigate in this work the presence of magnetic interaction at room temperature due to the interaction between the oxygen vacancies and the TM atoms. Measurements of SnO2 thin film with a magnetic field applied were also carried out to compare the results and to better understand the origin of the possible ferromagnetism.

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Self-assembled semiconductor/metal layers rolled-up microtubes for versatile applications and study of elastic properties of thin layers.

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The combination of deposition technique in which self-assembly is observed ant lithographic techniques has been widely used in present electronic devices as well as in development research for future technologies. Recently the deterministic releasing of thin films have attracted large interest due to the possibility of producing very thin membranes a plethora of materials [1], as well as for the fabrication of rolled-up semiconductor microtubes/nanotubes can be used as nano-reactors [2], resonant cavities [3], waveguides [4] and electronic devices [5]. In these structures the partial release of the layer strain also results in a change of the lattice configuration, modifying the material band structure and its optoelectronic properties [6, 7]. For this work, we report steps of production of rolled-up semiconductor structures consisting in a sequence of a 15-nm thick In0.2Ga0.8. As epitaxial, grown on top of an etchant-sensitive AlAs layer (20nm) on a GaAs(001) substrate. A metal layer is deposited by thermal evaporation on top of this semiconductor structure and an in-plane strain difference is obtained due to the induced surface tension. Selective etching of the sacrificial layer (AlAs) is then used to allow for rolling up. We are currently improving our tube production techniques, aiming for studying the elastic properties of additional very thin metallic layers and nano-objects that may be transferred to the top of the metal films prior to rolling.

Keywords: Rolled-up microtubes, strain release

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Silicon nanoparticles produced by laser ablation: morphological and optical characterization

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Different from bulk silicon, that presents poor luminescence because of its indirect gap, Silicon nanoparticles are known to yield intense light emission at visible and near-infrared regions. The success in synthesizing Si nanoparticles by laser ablation may open a lower cost, no-chemical route for obtaining semiconductor nanostructures. The present work reports on the fabrication and characterization of luminescent Si nanoparticles produced by laser ablation. Our two-step laser ablation process was performed in two different solutions, isopropilic alcohol (IPA) and acetone. First, usual ablation is done with the Silicon target immersed in the solvent, using a Q-switch Nd-YAG laser (1064 nm) with 200 ns pulses of 1 mJ with a repetition rate of 1 kHz, for 15 min. The second step is to submit this solution to an additional laser exposition, using the same laser parameters and times of 4 and 6 minutes. This causes a further fragmentation of the Si particles. High Resolution Transmission Electron Microscopy at 300 kV (HRTEM) measurements were performed, revealing nanoparticles tipically of the order of 7 nm or less for acetone and 20 nm IPA. Selected Area Diffraction (SAD) shows that the Si nanostructures are crystalline, independent on particle size. These nanocrystals are expected to emit light within the visible spectra. Micro-photoluminescence experiments were performed with a 532 nm laser focused by a 50x microscope objective, with particles deposited from the solutions onto a Si substrate. There is a slight difference between the light emission of nanoparticles in acetone and IPA solution. Nanostructures in acetone luminesce at 615 nm, while those obtained in IPA emit light at 650 nm. This difference can be explained by confinement effects since in the acetone solution the nanoparticles are smaller than in the IPA. The PL FWHMs are also different, being consistent with the wider nanoparticle size distribution for IPA samples (larger dispersion).

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Solar cell intended annealing effects on the optical, structural and electrical properties of commercial Indium Tin Oxide (ITO) thin films

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The indium tin oxide(ITO)is widely used as transparent conducting electrodes in optoelectronic devices due the great combination of optical transparency and electrical conductivity. The processes used to build TiO2 based hybrid and dye sensitized solar cells generally involve annealing or other thermal processes in order to optimize the ITO/TiO2 interface and/or induce TiO2 recrystallization. In this work we have explored the effects on the optical, structural and electrical properties of commercial ITO substrates when subjected to the main processes involved in the production of hybrid and dye sensitized solar cells. In special, 30-minutes subsequent annealing in ambient atmosphere were performed at different temperatures (25°C, 150°C, 300°C, and 450°C) using a 10 °C/min rate. Optical transmittance in 190-1100 nm spectral range, sheet resistance, and x-ray diffraction measurements were performed before and after each annealing process. The results of sheet resistance shows a significant decrease in electrical conductivity mainly after the 300°C and 450°C annealing, the sheet resistance values for these going from 15 $\Omega/$ up to 340 $\Omega/$. On the other hand, no systematic effects were observed on the spectral transmittance for all treatments. The x-ray diffraction also show only slight variations due to the annealing series, showing that there was no important structural or morphological modifications. The discussions concern the passivation of oxygen vacancies and others thermal activated defects, which are important for a good electrical conductivity.

Spatial distribution of the carriers wave functions on semiconductor quantum systems

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The confinement potentials of semiconductor nanostrucutres can be engineered to create different spatial distributions for the carriers. These distributions define important properties of the systems. For instance, the superposition of the carriers wave functions define the typical decay time of the excitonic state. As an illustration, on type II nanostructures for example, the two carriers do not occupy the same position, making the superposition small. This implies in a longer excitonic decay time when compared to type I systems. In the same way, other quantity determined by the wave functions is the activation energy, which is the energy needed to brake the excitonic state, for example, when the temperature is raised. In this work, we use a commercial package to calculate the carriers wave functions by numerically solving the Schrodinger equation. The advantages of this method are: i) the possibility to choose an arbitrary geometry, ii) include any known potential into the equation, iii) set different parameters to each material and iv) a visual and simple interface that makes it easier to have an insight when compared to traditional Fortran based algorithms. For the first problem, we chose an InP/GaAs type II semiconductor quantum dot, where the electron is confined in the dot and the hole is around it. We started with a simple model: a 2D quantum dot with a lens-shape geometry. We considered 3 contributions to the potential of the electron and hole: the confinement potential from the nanostructure, the strain contribution and the coulomb interaction potential. The hole can be confined only due to the last two contributions. The results of the wave functions show that the strain is already enough to localize the hole above the dot. The coulomb interaction completely determines its position, forming a ring over the dot for some specific geometries. This method has shown to be a powerful and simple one with possibility to study arbitrary geometries (pyramidal, conic, wires, wells, devices, etc. . . .) and other systems (stacked, uncapped, other materials). It can also be used with other differential equation based theoretical models.

Spin dynamics of carriers in p-i-p resonant tunneling diodes

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Spin dynamics of carriers in semiconductor devices is a fundamental issue for spintronic applications. In this work, we investigated this topic in p-i-p GaAs/AlAs Resonant Tunneling Diodes (RTDs) by measuring time-resolved polarized photoluminescence under magnetic fields parallel to the tunnel current. Under an applied bias, holes introduced by doping attain a quasi-stationary distribution along the structure, while photo-generated electrons are only created at the top GaAs layer during a pulse excitation by a ps - Ti:Sa laser tuned below the quantum well (QW) absorption edge. Subsequently, the electrons may tunnel into and recombine with holes at the QW. Therefore, the QW transient gives direct information on the spin dynamics of electrons tunneling through the structure. For bias around the resonance of the fundamental QW electron-level, we observed a very large polarization (60% at 15T) that is mainly constant during the whole transient and cannot be explained by the small Zeeman- splitting energy. The RTD structure thus seems to act as a spin-filter where electrons injected into the well acquire a preferential spin that is at least partially retained when they recombine. For other biases, the polarization shows a much complex dynamics, including sign inversions along the time-evolution of a given transient. Our results reveal that the structure provides different spin-polarization mechanisms with different characteristic times that may result in distinct spin polarizations of the carriers depending on the applied bias.

Spin filtering effects in InGaAsN/GaAs quantum wells

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In the last years, the spin manipulation was successfully realized in non-magnetic semiconductors nanostructures such as quantum wells (QW) and self-organized quantum dots. However, with increasing temperature up to room temperature (RT), free carriers get delocalized and their spin relaxation time drastically decreases. This limits the electron spin polarization under continuous-wave (CW) photoexcitation to few per cent. More recently, it was reported that spin-dependent recombination (SDR) processes via spin-filtering Gai self-interstitial defects can transform a nonmagnetic (In)GaAsN into an efficient spin filter operating at RT without applying a magnetic field. These processes provide conditions that are desirable for device applications. However, a systematic study of SDR has not been realized yet. In this work, we have investigated SDR effects in InxGa1-x As1-yNy / GaAs QWs as a function of temperature, laser intensity and QW width. Our samples consist of QWs of 4, 7 and 9 nm with x=36% and y=1.2% or y=0 (control sample) grown by molecular beam epitaxy on (100) GaAs substrates. We have measured polarized resolved photoluminescence by using circularly polarized excitation with wavelengths of 810 nm propagating parallel to the growth. Under such excitation conditions, most of the carriers participating in the optical recombination in the InGaAsN QWs were injected from the GaAs barriers and the cap layer. Both circular-polarization of excitation light and polarized resolved PL were obtained by using a quarter-wave plates together with linear polarizer. We have observed that the SDR effect becomes stronger in the wider QWs probably due to an increase in the sheet concentrations of the spin-filtering defects. In addition, when the temperature is increased, the polarization degree for N-free QWs decreases monotonically as a function of temperature. However, for N-containing samples the polarization increase up to 220 K. In conclusion, defect-engineered spin-filtering effects have been shown to be very effective for InGaAsN/GaAs QWs at room temperature especially for wider QWs.

Spin-assisted optical transitions in Zincblende quantum wells with two subbands

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In previous works we have developed a self consistent procedure to calculate the strength of the spin-orbit interaction for electrons in zincblende semiconductors by means of a folding down approach. In the process we have found a new contribution to the spin-orbit interaction arising from the distinctive parity of the quantum well eigenstates [Bernardes et al, PRL 99, 076603; Calsaverini et al, PRB 78, 155313]. Here we present a complementary discussion of the effects of renormalizing the electron wave function for the effective Hamiltonian. We find that this renormalization (i) shifts the energy levels of the quantum well, (ii) further renormalizes the in-plane effective masses, and (iii) does not change the spin-orbit interaction strength. We also discuss preliminary results on the direct optical transitions (within the conduction subbands) assisted by the interband spin-orbit interaction. In particular, we present an analytical expression for the imaginary part of the dielectric function of a symmetric quantum well. This work was supported by CAPES, CNPq, FAPESP, and the Research Support Center initiative of the PRP/USP.

Stability and electronic properties of Si- and C-terminated cubic SiC(001) surfaces

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Silicon carbide is considered to be a promising support material for heterogeneous catalysis and biosensors due to its low weight, high strength, extreme hardness, inertness and biocompatibility. In particular, the cubic β-SiC(001) surfaces, presents a number of stable different reconstructions offering carbon or silicon outermost layers with different stoichiometries, thus with different electronic properties when exposed to external ambient. However, little is known regarding the stability and reactivity of SiC surfaces to be considered in functionalization schemes. In this work we performed a systemathic study on the stability and electronic properties of C- and Si-terminated SiC(001) surfaces considering different reconstructions. Our ab initio calculations are based in the density functional theory and were performed using the VASP code within the asymmetric slab methods considering a c(2x2) periodicity for the C termination and both c(4x2) and (3x2) periodicities for the Si termination, including non-stoichiometric reconstructions. For C-SiC(001) we find seven stable stoichiometric terminations where four of them exhibit a dimer line formation and the two most stable present semiconductor characteristics. For the Si-SiC(001) we find eleven stable terminations where the most stable ones occur under non-stoichiometric Si-rich conditions, exhibiting dimer line formation. In addition we study the Fe adsorption and we observe that for the C termination the Fe atom is absorbed close to the C line and the system presents metallic and a ferromagnetic order.

Strain effects in InGaAs(N)/GaAs quantum wells along [001]

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In semiconductor nanostructured systems, composition, confinement, strain and magnetic fields have an important influence on electronic structure. Such effects result in peculiar behaviors once they are all combined simultaneously. It's also particularly interesting in dilute nitrides, where small amounts of N lead to drastic changes of the band structure, as for instance the strong renormalization of the energy gap. Actually, when a small fraction of As atoms in GaInAs is replaced by N, the energy gap of the material decreases by as much as 150 meV per N mole fraction (the so-called giant bowing effect). The reduction of the gap is attributed to the coupling between the bottom conduction band and the top of the resonant band of localized nitrogen [1]. Within the framework of a multiband calculation these effects can be combined to the strain contribution. We considered a biaxial strain produced at the interfaces that were subsequently introduced into the Pikus-Bir Hamiltonian [2]. In the calculations, the hydrostatic strain component renormalizes the gap (δEh) while the shear strain leads to the relative shift (δEs) between valence subbands, heavy and light-hole. The conduction and valence band energy levels were calculated for InGaAs/GaAs and InGaAsN/GaAs double quantum wells with 4 and 7nm grown along [001] direction. Our results show that the compressive strain (ϵ

Structural characterization of silicon nanoparticles produced by ball milling

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Nanometric semiconductor materials are currently being investigated because of both their potential for new technological applications and the interest in the fundamental physics of these systems. Silicon nanostructures present promising applications for production of optoelectronic and microelectronic devices, integrated circuits and information storage. This work reports the production of silicon nanostructures by using high-energy mechanical milling: a technique involving repeated grinding, welding and re-welding of a powder used as precursor. High purity silicon powder was submitted to the ball milling process in which parameters such as time of milling, mass and size of tools, were adjusted in order to control the dimensions and crystalline degree of the particles. By applying this process, it was possible reduce the dimensions of silicon particles to few dozen nanometers. Our samples were processed during 60 hours. In each step, the milling was stopped and the size distribution of the nanoparticles was determined through a particle size analyzer. These measurements were complemented by scanning electron microscopy images. Raman spectroscopy analyses were accomplished in order to study modifications in the material structure induced by the milling process.

Keywords: Silicon nanostrucutres, high-energy mechanical milling, Raman spectroscopy.

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Structural characterization of $Zn_{1-x}Co_xO$ thin films prepared by electron beam physical vapor deposition method

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The interest in Zinc Oxide (ZnO) doped with transition metal has been attracted much attention in the last years since it was predict a long range magnetic ordering above room temperature in such systems [1]. In spite of the extensive studies on Co-doped ZnO, the origin of its magnetic properties still remains a controversial issue. Some recent theoretical and experimental results have been shown that magnetic ordering depends on defects, such as oxygen vacancies, created during the sample preparation [2, 3]. Co-doped ZnO thin films were prepared via synthesized via Electron Beam Physical Vapor Deposition (EBPVD) with different Co molar concentrations of 1, 2 and 3%. The crystal structures of the samples were characterized using X-ray diffraction (XRD). The microstructure and composition distributions were characterized by scanning electron microscopy (SEM) and energy dispersive X-ray (EDS) measurements. RAMAN scattering was used to study of the incorporation of dopants and the resulting lattice disorder of the host lattice. Co K-edge x-ray absorption near-edge structure (XANES) and extended X-ray absorption fine structure (EXAFS) was used to determine the valence state and to evaluate the environment of Co in the ZnO lattice. Changes in the density of defects were estimated by RAMAN, Photoluminescence (PL) and HALL measurements. The conjugated different techniques confirmed the Zn replacement by Co ions in the wurtzite ZnO structure, which retains a high crystalline quality. No segregated secondary phases neither Co-rich nanocrystals were detected. However, the Co incorporation into the ZnO matrix introduces structure distortions and point defects that would be possible to lead to the desired ferromagnetic behavior.

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Structural properties of Co and $MnTiO_2$ nanoparticles analyzed by Raman scattering and x-ray diffraction

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Transition metals, such as Mn, Fe and Co, have been frequently used to dope large-bandgap semiconductors such as GaN, ZnO, as well as TiO_2, in order to introduce magnetic properties into systems, the so called diluted magnetic semiconductors (DMS). However, the origin of the magnetic properties from those materials is still a controversial issue. Therefore, correlations between magnetic and other material properties, such as optical and structural, are important for understanding these systems. In this work, we used Raman scattering and X-ray diffraction techniques to investigate the structural properties of the transition metals Co and Mn in $Ti_{1-x}TM_xO_2$ nanoparticles in samples prepared by the Pechini polymeric precursor method. We investigated three set of samples. For two sets, anatase is the dominant crystal phase, while for the other set, rutile is the dominant phase. In each set of samples, the Co and Mn concentration was varied from 0 to 0.12. X-ray diffraction patterns were refined by the Rietveld method. The analyses reveal a lattice parameter variation induced by the TM incorporation. X-ray measurements did not reveal secondary phase segregation, neither Co-rich nor Mn-rich nanocrystals. We believe that the signature of those effects should be below our experimental sensibility, even for high Co or Mn doping levels. Raman scattering results are consistent with the X-ray diffraction data. They show the same dominant phase established for each set of samples. The Raman frequency modes also shift with increasing TM content. In this case, however, the shift could be related to two distinct effects: i) change of the lattice parameter, and ii) variation of the average size of the $Ti_{1-x}Co_xO_2 or Ti_{1-x}Mn_xO_2$ nanoparticles. We discuss the possibility of these two contributions for our samples. The morphology of the samples and its grain size distribution was evaluated by transmission electron microscopy.

STUDY OF ELECTRONIC STRUCTURE OF CU2O IN THE PRESENCE OF CHLORINE IMPURITIES

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Cuprous oxide (Cu2O) has received attention for being an abundant, low cost and non-toxic semiconductor material with a direct band gap of 2.17 eV [1]. Furthermore, its natural conduction type is p, due to the existence of point defects in its crystal lattice. In order to apply it properly in electronic and photovoltaic devices, there must be a viable way to dope this material, turning it into n type. One possibility is the doping with chlorine atoms, that is effectively observed experimentally [2]. However, the electronic properties and mechanisms of this dopant remain obscure, thus requiring a more detailed theoretical study of the material [3]. Therefore, we have used the computational codes PWSCF/Quantum ESPRESSO, to perform electronic structure calculations based on density functional theory (DFT) using plane wave basis and pseudopotentials [4]. The calculations, with 2x2x1 supercells, had the objective to investigate the electronic properties of Cu2O in the presence of chlorine impurities, by obtaining formation and transitions energies, structural parameters (e.g. lattice parameter) and to determine carriers type. Five structures were considered: the stoichiometric cell, the cell with a copper vacancy, the cell with a chlorine impurity and the latter by adding a vacancy in two different positions. All the dopants were introduced substitutionally. Through a structural optimization, we observed changes in the values of lattice parameters of the defectives supercells, with an increase of this parameter for structures doped with chlorine. It was also found that vacancy coupled with chlorine impurity can exist and it is more stable than just the substitution of one chlorine by one oxygen.

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Study of undoped and Er-doped Nb2O5

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Niobium oxide Nb2O5 is increasingly applied in various modern technologies because of their unique physical properties like high refractive index (2.2 to 2.6), wide band gap(3.5eV), high dielectric permittivity (11 to 100) and good chemical and thermal stability. Particularly, the high index of refraction and the wide band gap, which is related to a low dielectric loss, are interesting issues for the use of Nb2O5 as a dielectric material for capacitor technology as well as a transparent material in optical systems. Additionally, the insertion of rare-earth ions in semiconductor matrices have been intensively investigated in the last years due to strategic interests of developing infrared lasers, amplifiers and up-conversion solar cells. Erbium (Er) is the most popular ion which has played an important role in the development of optical communications amplifiers around the region of low loss in optical fibers at 1.5 m. In this work, we have studied the synthesis and physical properties of undoped and Er-doped Nb2O5 samples prepared by Pechini method by X-Ray diffraction (XRD), Raman spectroscopy and Photoluminescence (PL). Nb2O5 samples present many crystalline phases which are strongly dependent on the preparation parameters. Particularly, we have observed that the synthesis temperature is a very important issue for the crystallographic properties. Our results show that the hexagonal phase dominates for samples prepared at 500 °C while the orthorhombic phase is increased for samples prepared at 600 °C. This result seems do not depend on the dilution precursor used for sample preparation. Concerning to Raman spectroscopy results we have observed for all samples a main peak at around 700 cm-1. This peak has showed a red shift for samples with different phases (hexagonal to orthorhombic phases). The formation of hexagonal phase is usually attributed to the small presence of oxygen during synthesis process. This fact was used to choose the hexagonal phase of Nb2O5 for Er-doping. Strong luminescence due to the I13/2 – I15/2 transitions of Er ion is observed which corroborates the absence of clusters. Comparison of structural and optical characteristics of undoped and doped Nb2O5 is under investigation.

Studying the properties of the alloy NiTi elastics

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The term EMF (Shape memory effect) used to describe the ability of certain materials,after having been plastically deformed by returning their original shape by heating. Normal alloy when deformed beyond its elastic limit has a permanent deformation plastic. Physically, the EMF associated with the transformation martensite cristalografic cally reversvel. that quality has stimulated research on materials that have higher rates of recovery and high temperature processing, since the increase in the number of papers presented in the literature current. A prominent place was given s-type alloys for many decades FeC relation with the SMA, when they discovered that other alloys may also show the same properties at rates Higher such as NiTi alloys known from the decade of the 70th, originally developed NASA to hidraulic engagement in military plane, has one of the best performances in terms of shape memory alloys (SMA), with recovery of form at 7%. materials metalics have this interesting property that are employed in various segments of metalurge industry, from aerospace to vo, eletronics, construction, Robotics and Bioengineering. This type of material can be used in connectors, sensors, safety devices, and many other applications. Another classification of dog EMF these types of materials are considered as materials intelligent, because they have self-correcting alterations in the behavior or function of time temperature. The aim of this study was to develop a methodology from first principles (DFT) to determine the parameters such as the cohesive energy (Ec) given elastics (C11, C12, C44) and distance to neighbors (ro), which are necessrias to adjust the potential interaction Classical, using a tight-binding aproximao of the 2nd moments that will be used in study systems via molecular dynamics, which contains alloys with EMF.

Tavis-Cummings model for two-exciton single-cavity systems with Coulomb and effective magnetic field interactions

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Semiconductor quantum dots embedded in a microcavity open the possibility to study cavity quantum electrodynamics in the solid state physics. One of the many interesting phenonema that is observed experimentally and have also been extensively studied theoretically is the coupling between an exciton in the quantum dot with the cavity modes. Coupling between two excitons and a cavity has also been observed. In this work, we present a numerical study of a two exciton system inside a single cavity, in the presence of a magnetic field, in the framework of a Tavis-Cummings model. The cavity considered is a semiconductor microcavity with a high quality factor. The excitons are considered as two-level systems and the external magnetic field is used to control the coupling parameters of the Hamiltonian. We calculate the dynamics of the system using the master equation in the Lindblad form, in the strong coupling regime between the cavity and the excitons. We include explicitly in the calculation the Coulomb interaction between the excitons. We modeled environments such as dephasing, exciton pumping, and incoherent loss of photons. Exact formulas for the time evolution of the density matrix and an approximation to the dynamics of the first excitation level were developed.

Thermoelectric transport in PbSnTe alloys

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There is an increasing interest in the search for new and efficient thermoelectric (TE) materials specially for applications in local cooling and exploitation of waste heat. The IV-VI semiconductor coumpounds, in particular PbTe, are among the most used and studied TE materials; however, with respect to PbTe, the PbSnTe alloy can have important advantages as lower thermal conductivity and better machanical stability, but has attracted much less attention. In this work we present a theoretical investigation of the PbSnTe TE properties. The PbSnTe electronic structure near the fundamental gap is obtained with Dimmock's multi-band kp model [1]. The electrical conductivity and Seebeck coefficient are then calculated with stardard solutions of the Boltzman equation, using different relaxation time approximations. Large variations in the TE power factor as a function of temperature, Sn concentration and electron density are obtained. The PbSnTe optimum temperature range and electron concentration for TE applications are discussed, and in particular the bipolar TE transport is shown to lead in general to significant contributions to the PbSnTe TE power factor.

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Thermoelectric transport properties throught two quantum dots: U finite atomic approach for the Anderson model

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We study a system of two quantum dots coupled to a conduction channel, taking into account a strong but finite Coulomb repulsion in each dot; we employ the impurity Anderson model and the U finite atomic approach for the model [1,2], without takes into account a direct coupling between the dots. We study three different systems: two dots inmersed into the conduction channel, a quantum dot inmersed into the conduction channel and the other side coupled to the conduction channel, and the two quantum dots side coupled to the conduction channel.

We compute the linear electrical conductance G, themopower S, thermal conductance K, and thermoelectric figure of merit Z as function of the dots energies, hibridization between the dots and the conduction channel, and temperature. Our results shows that the thermoelectric properties depends of the different quantum dots regimenes, and the geometric configurations of the system; we interpretate the results in terms of the different quantum interference process in the system and the indirect coupling between the dots, mediates for the conduction channel (RKKY interaction).

We look for the conditions that improve the thermal efficiency of the system, studing too the Wiedemman-Franz law.

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Time resolved photoluminescence studies of two-dimensional gases in a resonant tunneling structure

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Resonant tunneling diodes (RTDs) are interesting systems to study two dimensional gases (2D). The larger advantage of using such devices is that it provides the possibility of adjusting the 2D gas concentrations in a controlled way by varying the applied voltage. In addition, the 2D gases accumulated in RTDs plays a fundamental role on the spin polarization of the injected carriers, a fundamental point for potential applications of RTDs to spintronic devices [1]. In this work, we have performed time resolved photoluminescence as a function of the laser intensity and the applied bias voltage in p-i-p GaAs/AlAs RTD structures. Both parameters affect the concentration of the 2DHG and the electric field in the device. The results provide a rich set of information regarding the dynamics of the photocreated electrons and the 2DHG properties. Under applied bias, holes from the p-contact attain a quasi-stationary distribution in the RTD, including a 2D hole gas formed at the accumulation layer formed in the structure. Under light excitation, electrons are photocreated solely during the laser pulse. The photogenerated electrons can also tunnel into the quantum well (QW) and out of the QW to the contact, eventually recombining with holes at those different layers. Time-resolved PL thus gives relevant information on the complex dynamics of the minority photocreated electrons tunneling through the structure. We focus here on the emission around the GaAs band gap energy. By analyzing both the energy and the time-evolution of this emission range, we can discern the contribution of different transitions attributed to recombinations at the GaAs doped contacts and a 2D hole gas - free electron (2DHG-e) recombination. The later one is observed only around the first electron resonance assigned to the indirect Γ-X resonance. At this particular condition, the concentration of holes at the accumulation layer is already significant while the electric field is not too large yet, and the probability of the 2DHG-e is still considerable.

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Transmission reduction in branched out quantum rings

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Suppose you have a system where particles must go from a left channel to a right channel passing through two possible paths, just like in the case of a quantum ring attached to leads. Common sense says that if we add a third pathway, the transmission through the system must be enhanced. However, interestingly, shows both experimental and theoretical evidence that branching out a mesoscopic network does not always improve transmission. This effect was compared to the Braess paradox of games theory, but now on a mesoscopic scale. Besides, as they were dealing with a system consisting of wide transmission channels, quantum interference are expected not to be relevant.

We demonstrate that the transport inefficiency recently found for branched out mesoscopic networks can also be observed in a quantum nano ring with finite width attached to an horizontal branch. Our results show that the conductively of the ring does not necessary improves, if one adds an extra channel for electrons transport, this is shores that there exists a quantum analogue of the Braess Paradox.

Transmission Through Silicene Quantum Barriers

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Silicene is a monolayer of silicon atoms that form a two-dimensional honeycomb lattice similar to graphene's. It has attracted considerable attention due to its exotic electronic structure and its compatibility with current silicon-based electronic technology. The low-energy physics of silicene is described by Dirac electrons with relative large spin-orbit interacttions due to its buckled structure[1]. Its band structure can be controlled externally by an electric field. We explore resonant features in the electronic transmission through silicene-based barriers by theoretically studying it as a function of the electron's energy and its angle of incidence Θ. The incident electrons are assumed spin polarized and the barriers are formed by contact potentials. Our results show that the applied electric field may result in spin-resolved transmission channels. In addition, we critically compare the results with those through graphene-based barriers. Similar to graphene's case[2], the transmission is perfect for $\Theta = 0$ and shows a similar dependence on $\Theta \neq 0$ but important differences remain and are highlighted in the transmission and polarization.

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Transport of hole carriers in Pb1-xEuxTe alloys in the intrinsic regime in both sides of metal-insulator transition

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Conduction mechanisms in the temperature range of 250-450 K are investigated on p-type Pb1-xEuxTe films with Eu content x = 0%, 2%, 4%, 6%, 8% and 10% covering both sides of the metal-insulator transition that occurs around x = 6%. For samples with x = 0%, 2% and 4%, the electrical resistance increases as the temperature increases between 250 K and 330 K presenting metallic like behavior but, unexpectedly, the resistance starts to decrease as temperatures reach values higher than 330K. The analysis performed on the electrical resistance curves using the Differential Activation Energy method (DAE) revealed that this effect is originated from the intrinsic regime that occurs at high temperatures. This effect was not observed on previous results already published for p-type Pb1-xEuxTe films and we attribute this fact to the different growth conditions of the samples investigated in this work. In addition, for the insulating samples, the analysis using the DAE method shows that band conduction is the dominating conduction mechanism in the whole range of temperatures measured and agrees with previous results already reported. This is an indication that the insulating samples are less sensitive to modifications in the growth conditions than the metallic ones. These results bring additional information to the general picture of transport properties in p-type Pb1-xEuxTe films.

Keywords: Conduction mechanisms, PbEuTe, intrinsic regime, metal-insulator transition

Tunneling dynamics of carriers in p-i-n GaAs/AlAs double barrier diodes

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In this work, we have investigated the time and polarized emission of p-i-n GaAs/AlAs resonant tunneling diodes under magnetic field parallel to the tunnel current. Three resonant peaks were observed in the current-voltage characteristics curve (I(V)) and associated to the light-hole (LH1), electron (E1) and heavy-hole resonances (HH2). Under magnetic field, additional peaks due to scattering-assisted resonant magneto-tunneling are observed at higher voltages. Two quantum well (QW) emission lines were observed depending on the applied voltages. Under hole and electron resonance voltages the emission was dominated by an emission line at $\sim$1.61eV and $\sim$1.59eV, respectively. It was observed that the QW emission spectra present abrupt transitions between these two emission lines near electron and hole resonances. An optical bistability was observed for time resolved photoluminescence results. We have also studied the spin-dependent tunneling by analyzing the right ($\sigma+$) and left ($sigma$-) circular polarization from both, the contact layers and the QW electroluminescence as a function of the applied voltage and under magnetic fields up to 15T parallel to the tunnel current. We have observed that the QW polarization degree for the QW emission lines are highly bias sensitive and exhibit strong oscillations with values up to 80% at 15T. We also observed that emission from GaAs contact layers show evidence of spatially indirect recombination between free carriers and carriers confined in the two dimensional electron gas (2DEG) and hole gas (2DHG) . These emissions are voltage sensitive and highly polarized.

Tunneling phase time for electrons and holes through strained InP twin-plane nanowires.

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We prescribe appealing tunneling events both for electrons and uncoupled holes, traveling through a double barrier ($n = 2$ cells) and a superlattice ($n > 2$ cells) based on twin-plane nanowires. Motivated by the successful confirmation of surface effects on transparency modulation of these superlattices[1], we applied the Multicomponent Scattering Approach[2] to model further features of quantum transport in the same system. Our phase time (τ) simulation, shows several anomalous transport properties for involved charge carriers and averaged out, as expected, the mini-band spectrum for twin-plane 1D superlattices[1]. Direct proves of the paradoxical Hartman prediction[3] are investigated, looking for an autonomous behavior of τ, when topological parameters are broadened. The resonant Ramsauer-Townsend oscillations of τ, is also a subject of study, and several signatures of this phenomenon were found. Despite some criticism in the specialized literature, we report clear hallmarks of negative values for τ, as any numerical artifact had been accurately excluded. However the interpretation proposed here for this counterintuitive topic, a conclusive robust theoretical modeling remains a puzzle yet. Undoubtedly, such evidences are known and were reported elsewhere for electrons, holes and photon-twins in typical $III - V$ layered structures, but as far as we know they are novel events for twin-plane nanowires.

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Universality and the thermoelectric transport properties through semiconductor nanostructures

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We will discuss the temperature-dependent thermoelectric transport properties of semiconductor nanostructures comprising a quantum dot coupled to quantum wires, that is, the thermal dependences of the electrical conductance, thermal conductance and thermopower. The physics of electrical and thermal conduction through the nanostructures is controlled by the antiferromagnetic interaction between the magnetic moment of the dot and the spins of the conduction electrons in the wires. At low temperatures, the conduction electrons tend to screen the dot moment, which originates the Kondo effect. We explore the universality of the thermoelectric properties in the temperature range governed by the Kondo crossover. In this thermal range, general arguments indicate that the temperature dependence of any equilibrium property should be a universal function of the ratio T/T_K, where T_K is the Kondo temperature. Experimental work has nevertheless failed to identified universal behavior 1. On the theoretical front, the zero-bias electrical conductance through a quantum dot embedded in a quantum wire and the conductance through a quantum wire side-coupled to a quantum dot have recently been shown to map linearly onto the universal conductance for the particle-hole symmetric, spin-degenerate Anderson model 2. Here we extend this result to the other thermoelectric transport properties, the thermopower and the thermal conductance. Our analysis relies on rigorous renormalization-group arguments. Illustrative numerical renormalization-group 3 results will be presented to bring out the physics in our findings.

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Voltage controlled spin polarization of two-dimensional hole gases

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In the last years, there has been an increasing interest in the manipulation of spin degrees of freedom in semiconductor devices. In particular, some attention was focused on non-magnetic resonant tunneling diodes (RTDs) because the spin polarization of carriers in the structure can be voltage-controlled which is very useful for device applications. In this work, we have investigated the magneto-transport and circularly-polarized emission from the contact layers and the quantum well (QW) from p-type GaAs/GaAlAs RTDs as a function of applied bias and laser power, and under high magnetic fields (up to 15 T) parallel to the tunnel current. The I-V characteristics show various peaks that we assign to heavy-hole and light-hole resonances. The GaAs contact emission displays several bands including the indirect recombination between free tunneling electrons and holes localized at the two-dimensional hole-gas formed at the accumulation layer (e-2DHG). Both the energy position and intensity of this space indirect recombination are voltage-dependent. The degree of circular polarization from the GaAs QW and 2DHG-e emission are strongly sensitive to light excitation and bias-voltage. The Zeeman spin-splitting is also bias-voltage sensitive. The QW polarization degree exhibits large oscillations with a sign inversion around the heavy hole resonance. Our results show evidence that the spin-polarized hole-gas contributes to the circular-polarization degree of the carriers that accumulate at the QW.

Wave packet dynamics in semiconductor quantum rings due Braess paradox

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In recent years many sophisticated techniques of crystal growth have been used in several groups of research around the world in order to investigate optical, electronic, magnetic and transport properties of semiconductor materials. The interest in these structures has grown due to its applications in electronic devices and also because it has a chemistry procedure easily manipulated. In this work investigate the transport properties in a quantum ring semiconductor using the propagating of wavepacket like a gaussian packet to obtain the numerical results expected. We solved the equation of time-dependent Schrödinger using the technique known as split-operator, where it is applied to divide the time evolution operator into products of exponentials that do not commute, within the effective mass approximation. The investigated system consists of a quantum ring with the addition of an extra channel center. This system has been firstly investigated by the group of M. G. Pala [1] in a Mesoscopic system where it was proposed a comparison with the Braess paradox of game theory. The behavior that was experimentally observed was shown to be not trivial, because it was expected to increase the transmission coefficient, however this was not occurred. The system that we are investigating in this work has a different symmetry from that one proposed by M. G. Pala [1]. The ring structure studied by him has a geometry similar to a rhombus, while ours have a circular symmetry. Our results until the present moment show that for certain channel widths extra, implemented in the center of the system, improve the transmission coefficient, however for some values of the extra channel the transmission coefficient is reduced in its final value. This fact seems to be an intrinsic property of the system as a natural selection, exactly like it happens in the Braess paradox in game theory and in mesoscopic systems. Other observation is that when we change the width of the mean radius of quantum ring, there is a region where the transmission coefficient always exhibits a local minimum for the same value of the extra width of the channel, while for large values of the system this minimum is displaced as the average radius is varied.

Wave-packet scattering through a boundary monolayer and bilayer graphene

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Due to its unique electronic properties, graphene has become a topic of intensive study in recent years. Within the low energy approximation for the tight-binding Hamiltonian of graphene, electrons behave as massless Dirac fermions, with a linear energy dispersion [1]. This leads to a plethora of interesting physical phenomena as shown in recent papers that studied the scattering of electrons by edges and defects in graphene, both theoretically [2] and experimentally [3]. Electronic transport properties in monolayer, bilayer and at the interface between monolayer and bilayer graphene have also been studied [4, 5]. In this work, we study the electron transmission trough a boudary between monolayer and bilayer graphene. To do this we evaluate the scattering of a Gaussian wave packet at the interface between monolayer and bilayer graphene considering two types of graphene edges: armchair and zigzag. This theoretical investigation is made numerically solving the time dependent Schrödinger equation for the tight-binding model Hamiltonian, using the split-operator technique. Our purpose for this work is to calculate the transmission probability as a function of the incident angle of injected wave. The incident wave packet is calculated starting in the vicinity of the Dirac valleys K and K'. Therefore, we evaluate in which cases lead to valley polarization of transmitted wave packet.

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