Symposium N

POSTER SESSION PN1- Thursday, October 12

N501 - MAGNETIC STRUCTURE AND VOLUMETRIC MODULE THROUGH BANDS STRUCTURE CALCULATION OF Cr CARBIDES PRESENT IN HIGH LINKS STEEL

Carlos Alberto Kuhnen (UFSC), Jaoa Carlos Krause (URI) and Antonio Vanderlei dos Santos (URI)

For a better understanding of the compounds obtained by experimentation Cr_2C and Cr_4C, we calculated the electronic structure of both carbides in view of the fact that they are present in high links steels. For the performance of these calculations we used The Linearized Augmented Plane Wave (LAPW) with Generalized Gradient Approximation (GGA). Through these calculations we obtained the curve, the formation energy versus the volume in both cases, where we found a 353.65 a.u. equilibrium volume of ferromagnetic phase of Cr_2C and for the Cr_4C we found 368.43 a.u..

N504 - THEORETICAL STUDY OF METALLOPORPHYRINS OXO-DIMERS WITH METALS OF THE FIRST AND SECOND TRANSITION SERIES

Milan Trsic (IQSC-USP), Moacyr Comar Jr (UFAM) and Kelson Mota T Oliveira (UFAM)

In this work were analyzed the structural properties of metalloporphyrins dimmers, with transition metals, in which the monomers are aggregated through an oxo bridge. Five different basic structural conformations were found. The correlation of them with electronic structure of the monomers were observed. It was used the quantum method INDO.

N505 - THEORETICAL STUDY OF METALS AS POTENTIAL CATALYSTS IN HDS PROCESS

Reinaldo Rosberg E Garantizado (UFAM), Alexandre Mascarenhas Alecrim (UFAM), Moacyr Comar Jr (UFAM), Kelson Mota T Oliveira (UFAM), Carlito Souza Pedrosa (UFAM) and Jamal da Silva Chaar (UFAM)

Actually, the petroliferous industry investigates how to reduce the concentration of polluters in petroleum derivatives fuels, especially sulfur compounds as the DBT, 4-MDBT and 4,6-DMDBT through HDS process. This work use quantum mechanics to study the interactions among the 1st and 2sd transition metal series with the DBT and its derivatives. The approach used was Ab initio, with 3-21G* basis set, by Gaussian 03W package in PC platform.

N508 - DENSITY-FUNCTIONAL-THEORY CALCULATIONS OF CHARGED TORI CARBON ANOTUBE

Kelson Mota Oliveira (UFAM) and Moacyr Comar Junior (UFAM)

The theoretical study of carbon nanotube (CN) received great attention due the promise of its use in electronic devices. The investigation of the behavior of CN with additional charges and the effects of these charges on the electric potential generated are investigated in this work by use of DFT methodology.

N509 - CHANGE IN MAGNETIC AND ELECTRONIC PROPERTIES OF MNAS COMPOUND DUE TO SUBSTITUTION OF Mn BY Cr

Adelino Aguiar Coelho (Unicamp), Sergio Gama (Unicamp), Laudemir Carlos Varanda (Unesp), Miguel Jafelicci Junior (Unesp), Paulo Noronha Lisboa (Unesp), Momotaro Imaizumi (Unesp), Ariana de Campos (Unicamp) and Luana Caron (Unicamp)

The MnAs crystallizes with a hexagonal structure of NiAs a ferromagnetic phase and with orthorhombic structure MnP non- magnetic phase .We have simulated a new compound $(MnCr)_2As_2$ from MnAs compound by the substitution of one Mn atom by one Cr atom in a supercell with 4 atoms. We investigated the magnetic behavior of the new compound by studying its electronic structures with self-consistent spin-polarized energy band calculations, a full potential linearized augmented plane waves method (FP-LAPW), based on density-functional theory (DFT) and general gradient approximation (GGA).

N510 - HYDROGENATION OF ETHENE CATALYZED BY H-ZSM-5 MICROPOROUS MOLECULAR SIEVE: A THEORETICAL STUDY

Elton Santos Castro (LQC-UnB) and João Lopes Martins (LQC-UnB)

Zeolites are important class of aluminosilicates, with a three-dimensional framework, used as absorbents. Wide technological applications of zeolites justify the need of understanding their physical and chemical properties. Ethene hydrogenation is applied as a model reaction. Therefore it is important the understanding of catalyst effect for this reaction. The ONIOM3 method was used for the optimization of C_2H_4 and C_2H_6 molecules and the intermediate $-C_2H_5$. The calculations were performed using the GAUSSIAN98 program package. The cluster model with 576 atoms was used.

N511 - DESIGN OF MAGNETIC RADAR ABSORBERS USING GENETIC ALGORITHM

S C Raghavendra (UFPA), Jorge Andrey da Silva Macêdo (UFPA) and Victor Dmitriev (UFPA)

In this paper we report some theoretical results of multilayer radar absorber optimization. The absorber consists of several magnetic layers. The absorbers are optimized to obtain minimum thickness and maximum absorption. The e* and m* of magnetic materials selected in the optimization process are the experimental data from the literature.

N513 - WANNIER FUNCTIONS IN ONE-DIMENSIONAL CRYSTALS WITHOUT INVERSION SYMMETRY

Denis Rafael Nacbar (UNESP) and Alexys Bruno-Alfonso (UNESP)

We present a general procedure to obtain the best localized electronic Wannier functions of simple isolated bands in one-dimensional crystals which may lack inversion symmetry. They decay as a power law times an exponential and present the properties predicted by W. Kohn in the case of symmetric crystals. The theory is applied to describe electronic states in

semiconductor superlattices. We display the Wannier functions produced by different choices of the phase of the Bloch functions.

N517 - EXPERIMENTAL STUDY AND THEORETICAL MODELING OF THE PHOTOLUMINESCENCE IN DISORDERED Mn-DOPED $BaTiO_3$

Paulo Sergio Pizani (UNESP), Maria Aparecida Zaghete (UNESP), Miryan Rincon Joya (UFSCAR), Ieda Lucia Rosa (UFSCAR), Adaci Batista Campos (UNESP), Jose Waldo Espinosa (UFPb), Maria Fernanda Gurgel (UNESP), Jose Arana Varela (UNESP) and Elson Longo (UNESP)

This work report periodic mechanic quantum ab initio and experimental study te nature of visible photoluminescence (PL) at room temperature in amorphous BT:Mn , The results indicated that PL changes with the degree of disorder in the BT:Mn powders and suggests the creation of localized states in the disordered structure.

N518 - PERIODIC FIRST-PRINCIPLES CALCULATION OF SEMICONDUCTOR ZnO

João Batista Martins (UnB), Naiara Letícia Marana (UNESP) and Júlio Ricardo Sambrano (UNESP)

Periodic density functional theory has been carried out in order to determinate the structural and electronic properties for rocksalt, zinc blende and wurtizite ZnO. The periodic calculations have been carried out by means of the CRYSTAL03 computer code. An optimization procedure of the lattice parameters has been performed to minimize the total energy with respect to unit cell. Structural parameters and band structures are reported and compared with previous experimental data. B3LYP approach gives accurate account of structural and electronic properties of ZnO.

N519 - APPLICATION OF PREISACH'S MODEL IN ELECTRICAL STEELS MODELING

Nelson Jhoe Batistela (UFSC), Claudenei Simao (UFSC), Nelson Sadowski (UFSC), Willian Torazo Hamada (UFSC) and Joao Pedro Assumpção Bastos (UFSC)

Accurate hysteresis phenomena modelling is very useful in prediction of hysteresis losses. In this work, the Preisach's model is used to represent hysteresis phenomena under sinusoidal and non-sinusoidal voltage waveforms. A numeric program able to predict the magnetic material behavior under these conditions was developed. Calculated hysteresis loops are compared with experimental ones.

N520 - THE SM DOPING INFLUENCE IN THE STRUCTURE OF THE PBTIO3: THEORETICAL MODELING AND EXPERIMENTAL STUDY

Elaine Paris, José Waldo Espinosa (UFPB), Maria Fernanda Guergel (UFSCar), Antonio Zousa, José Varela (IQ UNESP) and Elson Longo

This work report periodic mechanic quantum ab initio and experimental structural deformation study caused by the Sm element in the structure of annealing $PbTiO_3$ obtained by polymeric precursor method. On the doping simulation the Sm element is not included but is possible to observe its influences on the structural distortion, the electronic density respond and atomic orbital distribution analysis of the PT samples. The subtle structural differences lead to perturbations in the crystal orbital splitting that allowed to characterize the disorder observed experimentally on these compounds.

N521 - THEORETICAL AND EXPERIMENTAL STUDY OF ELECTRICAL CHARACTERISTICS OF THE ORGANIC MOLECULE 4 – (O - OXY - P - PHENYLENE) – N – METHYL - 1, 8 - NAFTALIMIDE (NPPOX)

Eduardo Triboni (USP - São Carlos), Francisco Nart (USP - São Carlos), Gustavo Baldissera (UFPR), Marcos Allan Reis (UFPA), Jordan Del Nero (UFPA) and Lucimara Roman (UFPR)

The organic molecule NPPOX has been investigated by calculations and experimental methods to understand the geometric and electronic properties, first using Hartree-Fock derivative methodology modified to including electric field1 and after manufacturing a thin film devices by spin-coating. The results suggest that this molecule show strong semiconductors characteristics.

N522 - INDIVIDUAL CONTRIBUITION OF THE MATRIX AND TRIGLYCERIDES TO BAN-GAP OF BURITI OIL: POLYSTYRENE BLENDS

Geraldo Magela (I.Física - UnB), João Batista Lopes Martins (I. Química - UnB), Elton A Castro (I. Química - UnB), Maria José Araujo Sales (I. Química - UnB), Jussara Angélica Durães (I. Química - UnB), Ricardo Gargano (I.Física - UnB) and Artemis Marti Ceschin (Dep. Elétrica - UnB)

Buriti oil was blended with polystyrene yielding to hybrid materials with interesting thermal and optical properties, e.g. absorption and emission of light. This work presents a theoretical study about the contribution of the matrix and some triglycerides of the oil, based on the mainly fatty acid: oleic and palmitic.

N523 - EMISSION QUANTUM YIELD OF NEW LUMINESCENT LANTHANIDES COMPLEXES

Kenneth Raymond (University of California), Amanda Samuel (University of California), Ana Carolina Roma (UFPE) and Ricardo Luiz Longo (UFPE)

The optical properties of lanthanide compounds have important technological applications. These properties are directly related to the 4f-4f transitions within a 4f electronic configuration and to the coordinating environment. The experimental emission quantum yield and spectroscopic calculations of new luminescent lanthanides complexes are reported and the effects of the substituents in the organic ligands upon the excited states were investigated in order to optimize the energy transfer from the ligands to the lanthanide ion.

N524 - DFT PERIODIC STUDIES ON PLATINUM BULK

Antonio Carlos Dias Ângelo (UNESP/Bauru), Gustavo Franklin Nóbrega (UNESP/Bauru), Leandro Moreira de Campos Pinto (UNESP/Bauru) and Júlio Ricardo Sambrano (UNESP/Bauru)

Density functional theory (DFT) applied to periodic quantum-mechanical system has been carried out with B3LYP, PBE exchange-correlation and PWGGA exchange-correlation functional, by means of the CRYSTAL98 computer code in order to understand in a profound way the structural and electronic properties on Platinum bulk. The calculated lattice parameters,

band structure and density of states are reported and compared with previous theoretical and experimental data. The results are in good accordance with those one reported in the literature.

N525 - COMPARISON BETWEEN SIMULATIONS AND MAGNETIC MEASURES

Abio Valeriano Andrades Pinto (UFSC),
Tiago Jacques Schmidt (UFSC) and Agonir Wenginowicz (UFSC)

In this work we present a comparative study between simulation and experimental measures, where using dedicated software and a Hall probe we got a radial profile of a permanent magnet cylindrical. Of the confrontation of these experimentally generated data and for simulation presented, the experimental support seems to give credit to the simulated inquiry.

N528 - KAOLINITE AS HEAVY METAL REMOVER: A THEORETICAL STUDY

João Lopes Martins (LQC-UnB) and Elton Santos Castro (LQC-UnB)

Experimental results had shown that kaolinite can be used to sorb heavy metals as Cd, Pb, Zn, etc. This work studied the interaction energy of metals with hydroxyl and oxygen surfaces of kaolinite through methods as ONIOM2 (RHF/3-21G** : UFF), as well as the charge distribution of these complexes.

N529 - SnO_2 NANOSTRUCTURES

Júlio Ricardo Sambrano (Unesp/Bauru), João B. L. Martins (IQ/UnB),
Sandra V. da Silva (IQ/UnB) and Elson Longo (Unesp/Araraquara)

Tin oxide is a semiconductor of n-type with a band gap of 3.6eV. One of most used tin oxide crystallizes in the tetragonal rutile type structure. Tin oxide surfaces is an important material used in bioavailability of contaminant in environment, gas sensors and catalyst. Most recently, SnO_2 nanostructures have been reported. Theses studies shows that nanoparticles of this oxide has been used for the formation of nanowires growth along the most stable [110], [001] and [010] directions. The SnO_2 structure was calculated using B3LYP hybrid DFT method using the periodic Crystal98 program.

N531 - EVALUATION OF MECHANICAL PROPERTIES OF POLYAMIDES USED IN RAPID PROTOTYPING

Marcelo F. Oliveira (CenPRA), Izaque A. Maia (CenPRA), Jorge Vicente Lopes da Silva (CenPRA), Christiane Laranjo Salgado (UNICAMP),
Elisabete Maria Saraiva Sanchez (UNICAMP)
and Cecilia A.C. Zavaglia (UNICAMP)

Rapid Prototyping and Manufacturing technologies have emerged for quickly creating 3D products directly from computer-aided design systems. These technologies significantly improve the present prototyping practices in industry. On this study we evaluate the tensile properties of the new and recycled polyamide specimens molded on diverse directions, with the ASTM D638-02a standard. We also evaluated the degradation rate of the material using a thermo-gravimetric test (TGA) and the hardness with a durometer shore D.

N532 - INFLUENCE OF MN ON THE PRECIPITATION OF INTERMETALLIC PHASES IN $AlFe_4Si_4$ ALLOY

Walter José Botta Filho (UFSCar), Claudio Shyinti Kiminami (UFSCar),
Carlos Rios Triveño (UFSCar), Margareth Spangler Andrade (CETEC),
Elenice Cavichioli Borba (CETEC) and Claudemiro Bolfarini (UFSCar)

The influence of Mn on the precipitation of intermetallic phases in an $AlFe_4Si_4$ alloy is presented. The samples prepared by arc-melting and characterized by scanning electron microscopy, atomic force microscopy, differential scanning calorimetry and X-rays diffraction. The experimental results were compared with thermodynamic calculations fot the Al-Si-Fe and Al-Fe-Si-Mn system using the CALPHAD methodology (Calculation of Phase Diagram). The role of the alloy chemistry on its microstructure was -Al_3M (M=Fe,Si,Mn) were -Al(FeMn)Si, Si and -Al(FeMn)Si, analysed. The phases formed.

N533 - THERMODINAMICAL PROPERTIES OF SI AND SIC NANOWIRES

Lucy Credidio Assali (Instituto de Física - USP),
João Francisco Justo (Escola Politécnica - USP)
and Rafael Dias Menezes (Escola Politécnica - USP)

This work provides a theoretical investigation on the structural and thermodynamical properties of SiNWs and SiCNWs using molecular dynamic simulations and interatomic potentials. We considered nanowires with several diameters and <100> and <110> growth directions belonging, respectively, to Fd3m and F43m space groups. The stability in terms of nanowires energetics have investigated for each growth direction and diameters. Additionally, we have investigated the melting of nanowires as function of morphology, and established a scaling law between the melting temperature and the wire diameter.

N535 - INTENSE BLUE PHOTOLUMINESCENCE IN STRUCTURALLY DISORDERED $SrTiO_3$: SM

José Arana Varela (IQ - UNESP), Ederson Carlos Aguiar (IQ - UNESP),
Alexandre Zirpoli Simões (IQ - UNESP) and Elson Longo da Silva (IQ - UNESP)

Much attention has been focused in visible photoluminescence (PL) at room temperature in disordered materials due to their potential technological application on the development of new luminescent materials which includes compact laser devices operating in the blue region. Blue photoluminescence emission in structurally disordered $SrTiO_3$:Sm powders was observed at room temperature with laser excitation at 350.7 nm, for the first time. A joint experimental and theoretical indicate that the generation of the broad PL band is related to order-disorder degree in the perovskite-like structure.

N536 - ANALYSIS OF UNCERTAINTY IN THE PROCESS OF CHARACTERIZATION OF VISCOELASTIC MATERIALS

Pablo Rodrigo Medeiros (UFSC), Edison Rosa (UFSC)
and Antonio Brito Neto (UFSC)

This paper shows an approach about the questions involved in the uncertainty analysis in the rocess of haracterization of viscoelastic materials.

N539 - COEFICIENT DETERMINATION OF HEAT TRANSFER

Mírian de Lourdes Noronha Motta Melo (USF), Rezende Gomes dos Santos (UNICAMP), Marco A. Eid (UNICAMP) and Ana dos Santos Albert (USF)

The objective of this work is the implementation of a numeric model for the simulation of the solidification with radial heat flux capable of determining the main thermal and microstructural parameters and the coefficient of heat transfer in the metal/mold interface. The results of the model are validated with experimental results of an aluminum alloy. The results of this work provide important information for the modeling of the heat transfer in the solidification/casting process with radial heat flux.

N540 - ACTIVE SITES FOR PYRIDINE ADSORPTION

José A. Dias (IQ/UnB), Valdeilson S. Braga (IQ/UnB), Ivoneide C. L. Barros (IQ/UnB), Aline B. L. Gusmão (IQ/UnB), Silvia C. L. Dias (IQ/UnB) and João B. L. Martins (IQ/UnB)

A major scientific and technological achievement has been the discovery of synthetic crystalline aluminosilicate zeolites used as molecular sieve adsorbents and catalysts. It is well known that Bronsted acid chemistry is a dominant feature of the catalysis by zeolites in many important industrial applications, such as refining. Computational chemistry is a useful tool in order to study the active sites on zeolites and supported catalysts. We have used ab initio quantum chemistry method in order to calculate the vibrational frequencies of pyridine adsorbed on Al_2O_3, SiO_2, Al_2SiO_5, and Nb_2O_5.

N543 - ELASTIC MODULLI AND ELECTRONIC PROPERTIES OF $BaZrO_3$: PERIODIC DFT STUDY

Aguinaldo Robinson de Souza (UNESP), Melissa Cristina Tonelli (UNESP), Prescila Glaucia Christianini Buzolin (UNESP) and Júlio Ricardo Sambrano (UNESP)

Many research groups have devoted considerable attention on the development of ceramics with technological applications, especially the $BaZrO_3$. Density functional theory applied to periodic system has been carried out in order to determinate structural, electronic properties and the elastic moduli. The results are in agreement with experimental and theoretical data.

N544 - $BaTiO_3$: STRUCTURAL AND ELECTRONIC PROPERTIES WITH A DFT PERIODIC STUDY

Julio Ricardo Sambrano (Unesp-Bauru), Aguinaldo Robinson de Souza (Unesp-Bauru) and Melissa Cristina Tonelli (Unesp-Bauru)

Structural and optical properties of the cubic $BaTiO_3$ have been investigated by means of density functional theory with B3LYP and B3PW functional. The calculated minimal band gap is direct and indirect for B3PW and B3LYP, respectively. The results are discussed and compared with available experimental and theoretical data.

N548 - THEORETICAL INVESTIGATION OF TETRATHIAFULVALENE POLYMERS

Francisco Carlos Lavarda (D.Fisica-UNESP-)

Tetrathiafulvalene (TTF) and its derivatives are organic molecules that are frequently present in highly conducting or superconducting compounds. We investigated that configurations that would fulfill the conditions in which a TTF polymer would be an intrinsic one-dimensional conductor, according to these two rules: the polymer should have a two-fold screw S_2 symmetry axis and the unit cell should have $4N^{+2}$ electrons. The geometry is obtained with the semiempirical method Austin Model 1. Our conclusion is that the rules for the intrinsic conductivity can not be obeyed by TTF polymers.

N549 - MOLECULAR DYNAMICS OF A SINGLE WALL CARBON NANO-CANNON (SWCNC)

Luiz Antônio Pecorare Xavier (USJT) and Jordan Del Nero (UFPA)

Based on the Rutherford's Experience model, we had use a carbon nano-cannon shooting a probe into a gold wall. Motivated by the possibility in finding new forms and applications, we have designed a hypothetical single wall carbon nano-cannon. It will be ideal in study the elastic and plastic deformation behavior of some materials, under bending loads. In particular, various levels of studies were performed on the properties of the swnt's structure, including use of classical molecular mechanics (MM), molecular dynamics (MD) and mechanical properties as a function on the power to shot a probe.

N551 - BREWING A NEW MESOSCOPIC SCALE APPROACH TO SEMICONDUCTOR PHYSICS WITH HIGH PERFORMANCE COMPUTING: A SUCCESFULL CASE

Guilherme Matos Sipahi (IFSC - USP), Elton Marcio dos Santos (IFSC - USP), Marcel Nogueira Eurydice (IFSC - USP) and Ivan Paganini Marin (IFSC - USP)

In the search for new materials in solid state physics, high performance computing proved to be fundamental to tackle the ever-growing size and complexity of the problems. We present here the results of our development of simulations for several semiconductor materials, including diluted magnetic semiconductors (DMS) and Quantum Dots, using an effective mass (k.p) band model.

N552 - THEORETICAL STUDY OF STRUCTURAL ORDER-DISORDER IN CATIO3

Sergio de Lazaro (UFSCar), Rafael Luiz Erlo (UFSCar) and Elson Longo (UNESP)

Photoluminescence phenomenon in materials $ATiO_3$ have been studied experimental and theoretically in the literature. These materials can be an alternative to applications in optical devices and therefore a structure eletronic study is important to understanding the mains conditions to presence of this effects.

N553 - STUDY THEORETICAL ABOUT ADSORPTION OF O2 MOLECULE IN BATIO3 (001)

Armando Béltran (UJI), Júlio R. Sambrano (UNESP), Sergio de Lazaro (Ufscar), José A. Varela (UNESP) and Elson Longo (UNESP)

Adsorption of O2 molecules in the material TiO2 is known in the literature. However, adsorption of this same molecule in materials as BaTiO3 (BT) has been study more recently. This work investigated theoretically the

adsorption of O2 molecule in the material BT (001) with TiO2 termination and the O2 molecule in top. In there models are considerer that all the sites of Ti are occupied in the two faces and the molecule of oxygen has adsorption in the vacancies of Ti atoms. CRYSTAL98 program was used to the ab initio calculate of the properties electronics and structures to all the models.

N555 - ELECTRONIC STRUCTURE AND LOCAL MAGNETIC PROPERTIES OF TRANSITION METAL NITRIDES

João Carlos Krause (URI) and Juliana Zottis (URI)

The nitrides have been investigated with increasing interest in recent years, considering its promising technological applications. In this work, the DVM method is applied to calculate the electronic structure and magnetic properties of the nitrides Co4N, Mn4N, Ni4N, Sc4N and Ti4N. A somewhat large magnetic moment was obtained for the face centered site in the Mn4N compound (M_B=-1.22M_B). At the N site of the composites Ti4N, Sc4N, Ni4N and Mn4N, our calculations indicate that it acts as a receptor for electrons, whereas for Co4N the nitrogen acts as a donor.

N558 - STRUCTURAL AND ELECTRONIC PROPERTIES OF LITHIATED SnO_2. A PERIODIC DFT STUDY

Lithiated SnO2, which is envisaged to be an important system for anodes in Li-ion cells, has been investigated by periodic DFT calculations at PW91 level. Optimized structural parameters, cohesive energy, density-of-states, Mulliken population and open circuit voltage (OCV) for Li_xSnO_2 ($0 < x < 1$) systems are reported. The results render that Li 2s orbital is spread out in a region of 4.0-8.0 eV above the Fermi level, which implies that lithium essentially remains ionized in the oxide. In addition, Li intercalation is proved to induce metallicity.

N560 - CONFORMATIONAL STUDIES OF CHITOSAN BIOPOLYMERS

Francisco Carlos Lavarda (UNESP/Bauru)
and Nélio Henrique Nicoleti (UNESP/Bauru)

The main purpose of this work is to find the stable geometries of chitosan biopolymers through electronic structure calculations. Applications of chitosan are many, generally of strong impact and all apparently originated form its capacity to bind other substances in its chain. The geometry is obtained at the semiempirical level of theory, using the Austin Model 1 (AM1) hamiltonian, in vacuo and an aqueous environment. It is possible do conclude that the properties of the polymer can be reproduced from oligomers with 8 monomers.

N561 - COMPUTER MODELLING OF TRIVALENT METAL DOPANTS IN LITHIUM NIOBATE

Romel M Araujo (Univ. Fed. de Sergipe, BR), Robert A Jackson (Keele Univ, UK) and Mário E G Valerio (Univ. Fed. de Sergipe, BR)

Computational modelling, based on energy minimisation and the Mott-Littleton approximation, were used to study the doping porcesses by Sc Cr Fe and In in $LiNbO_3$. The dopants can substitute at both Li or Nb cationic sites and a range of different charge compensation schemes were considered. Solution energies were calculated at 0 and 293K. The lowest energy solution scheme was found to involve doping at the Nb site, with Nb-Li antisite charge compensation. The implication of these results in interpretation of the observed experimental properties of the doped materials is discussed

N562 - COMPARATIVE THEORETICAL STUDY OF STRUCTURAL AND ELECTRONIC PROPERTIES OF CARBON NANOTUBES AND FULLERENES, C20-C80

Greta Tami Araújo da Silva (UFAM/Química),
Cleuton Souza Silva (UFAM/Química), Kelson Mota T. Oliveira (UFAM),
Zuanny da Silva Jucá (UFAM/QPN) and Moacyr Comar Jr (UFAM)

The nanostructures have caused a great interest in the scientific community, for its amazing properties. This work, through computational molecular modeling, obtained structural and electronic properties from nanotubes of carbon and fullerenes. These data had pointed the hemispherical regions of the nanotubes as the most reactive part of the molecules and others interesting results. These molecules had been shaped and constructed using molecular quantum mechanics, in Hartree-Fock ab initio level, using 3-21G basis set, by Gaussian 03W package in PC platform.

N563 - CRITICAL CURRENT OF SUPERCONDUCTING FILMS WITH ARTIFICIAL PERIODIC PINNING CENTERS

Denise Fernandes de Mello (Unesp), Pablo Antonio Venegas (Unesp),
Rafael Plana Simões (Unesp) and Daniel Rodrigo Falconi (Unesp)

In our work we analyze the effects of artificial pinnings centers on the critical current of superconducting films using Molecular Dynamics technique. We solve the Langevin equation, which include the vortex-vortex, vortex-pinning and vortex-external current interactions. We analyze the hexagonal and Kagomé commensurate distribution of pinning centers for several densities of vortices and pinnings. Our results show that triangular is more effective than the Kagomé lattice to pin the vortices and the effectiveness of the pinning mechanisms decreases as the vortex density is increased.

N564 - HYPERPOLARIZABILITIES OF DONOR-ACCEPTOR DIETHENYLSILANE OLIGOMERS

Ramon A. Brennand (UFPE) and Ana Elizabete de A. Machado (UFPE)

Donor-acceptor diethenylsilane oligomers were theoretically investigated to optimization of the nonlinear coefficients. Calculations of static and dynamic β and γ hyperpolarizabilities were performed by using of AM1/TDHF methodology.

N565 - THEORETICAL STUDY OF NONLINEAR OPTICAL PROPERTIES OF SUBSTITUTED ANILINE OLIGOMERS

Ana Elizabete de Araújo Machado (UFPE)
and Marconi Bezerra da Silva Costa (UFPE)

Aniline substituted oligomers (trimers, hexamers) with halogens atoms (F, Cl, Br and I) were theoretically investigated to optimization of their nonlinear coefficients. Calculations of the static and dynamic β and γ hyperpolarizabilities were performed by using the semiempirical techniques AM1/TDHF. The three forms of the polyaniline (emeraldine, pernigraniline and leucoemeraldine) were considered in this work.

N566 - THEORETICAL STUDY OF NONLINEAR OPTICAL PROPERTIES OF DONOR-ACCEPTOR ANILINE OLIGOMERS

Marconi B. da Silva Costa (UFPE)
and Ana Elizabete de A. Machado (UFPE)

Donor-acceptor aniline oligomers (tetramers, octamers) were theoretically investigated to optimization of their nonlinear coefficients. Calculations of the static and dynamic β and γ hyperpolarizabilities were performed using semiempirical techniques AM1/TDHF. The three forms of the polyaniline (emeraldine, pernigraniline and leucoemeraldine) were considered in this work.

N569 - FIRST HYPERPOLARIZABILITY OF TETRAETHYNYLETHENE DERIVATIVES

Karina Anunciada Barros (UFPE)
and Ana Elizabete de Araújo Machado (UFPE)

Tetraethynylethene derivatives were theoretically investigated to optimization of the first hyperpolarizability(β). Donor and acceptor groups of electron were introduced in the systems designed for to enlargement of the βnonlinear response. Calculations of static and dynamic β hyperpolarizability were performed by using of the AM1/TDHF methodology.

H525 - DIELECTRIC PROPERTIES OF CZT THIN FILMS PREPARED BY CHEMICAL SOLUTION DEPOSITION

Sérgio Cava (UEPG), Iêdo Alves Souza (Unesp), Alexandre Zirpoli Simões (Unesp), Laécio Santos Cavalcante (Unesp), Luiz Ferreira Lima Jr (Unesp), Elson Longo (Unesp) and José Arana Varela (Unesp)

The $Ca(Zr_{0.05}Ti_{0.95})O_3$ (CZT) films annealed at 928K for 4 hours were grown on $Pt(111)/Ti/SiO_2/Si(100)$ substrates by the chemical method. CZT films present orthorhombic structure with a crack free and granular microstructure. Dielectric constant and dielectric loss of the films was 212 at 100 kHz and 0.032 at 1 MHz.

N570 - VISUALIZATION OF FRACTURE SURFACE IN 3 DIMENSIONS

Luis Rogerio de Oliveira Hein (FEG-Unesp), Arnaldo Homobono Paes de Andrade (Ipen), Raquel de Moraes Lobo (Ipen)
and Gerson Marinucci (Ipen)

Observations of materials and components fracture surfaces are accomplished, in general, through two-dimensional images (2D), resulting in loss of important information for a more necessary detailing of that area. The knowledge of the real topography of those surfaces can produce precious information for the understanding of the mechanisms involved in the phenomena of fracture. Three-dimensional reconstruction (3D) of those fracture surfaces, accomplished through the obtaining of a stereo pair of images by optical microscopy (OM) or by scanning electron microscopy (SEM), it can become a pow

N571 - GERMANIA – SILICA SUPERTETRAHEDRAL NANOPOROUS SOLIDS: COMPUTATIONAL STUDY OF SIMPLE POLYMORPHS

Marleny Rodriguez-Albelo (University of Havana), Angel Rabdel Ruiz-Salvador (University of Havana), Ariel Gomez (University of Guelph) and Dewi W. Lewis (University College London)

Hypothetical pure and Ge-doped silica supertetrahedral nanoporous solids are studied by computer modeling techniques. Pure silica polymorphs are used as templates for constructing the extended framework solids. The inclusion of Ge atoms favors the stress release caused by its presence on 3 member rings. In order to estimate the possibility of incorporating Ge into the framework the substitution energies are compared with those calculated for experimentally known Ge rich zeolites. The possibility of extending the design and prediction to more open zeolite-like solids is discussed.

N573 - STUDY OF SUPERFICIAL COATINGS BEHAVIOUR BY NUMERICAL ANALYSIS OF INDENTATION TESTING

Geralda Cristina Godoy (UFMG), Vânia Velloso Silva (UFSJ), Avelino Silva Dias (UFSJ) and Paulo José Modenesi (UFMG)

This work simulated the indentation testing behaviour of a rigid indentator on a coating/substrate system through FEM. Recently, many researchers have developed techniques which make use of this testing to evaluate material mechanical properties and also to characterize and analyze superficial coatings adhesion. It was obtained numerical results for the stress and strain fields, mainly for the indentator contact region and for the coating/substrate interface during the indentation cycle. Through the maximum main stress field it could get information about the coatings failure mechanism.

N574 - THEORETICAL SIMULATION OF STRUCTURAL PROPERTIES OF POLYANILINE FILMS

Rodrigo Ramos da Silva (IFUSP), Liliana Yolanda Dávila (UFT) and Marília Junqueira Caldas (IFUSP)

We study the structural properties of two types of polyaniline films, leucoemeraldine and emeraldine. The use of classical methods for geometry optimization allowed us to obtain results for the geometry of the films olygomers as well as the radial distribution function and X-rays diffraction spectra.