3RD BRAZIL MRS MEETING

October 10-13, 2004

S Y M P O S I U M F:

COMPUTATIONAL SIMULATION AS A TECHNIQUE TO DESIGN NEW MATERIALS

Symposium Organizers:

Júlio Ricardo Sambrano (DM - Unesp-Bauru)

João Batista Lopes Martins (DQ – UnB)

Rogério Custodio (IQ - Unicamp)

Fabrício Ronil Sensato (Fundação Santo André - SP)

COMPUTATIONAL SIMULATION AS A TECHNIQUE TO DESIGN NEW MATERIALS

Tuesday, October 12

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Session Chair: Ricardo Longo (DQF – UFPE)

08:00 MAGNETIC MOMENTS AND HYPERFINE FIELDS OF 4d IMPURITIES AND MONOLAYERS IN BCC IRON
C. Paduani. Fisica, UFSC, SC, Florianopolis, Brazil; J. C. Krause. DCET-URI, Santo Angelo, RS, Brazil.

08:15 MAGNETIC PROPERTIES OF CO_2MnX (X= Al, As) INTERMETALLIC COMPOUNDS AT ZERO AND ELEVATED PRESSURE.
I. Momotaro, J.F. Miguel, V.C. Laudemir. Unesp. Departamento de Física - Av. Emgenheiro Luiz Edmundo Carrijo Coube S/N- Bauru-SP- Brazil - Po BOX 473 - 17033-360; L. Bernardo, A.A. Alexandre, G. Sérgio, C.de A. Adelino, M.A. Marilsa. UNICAMP.

08:30 TEMPERATURE AND SALT CONCENTRATION EFFECTS ON THE STRUCTURE OF POLYMER ELECTROLYTE PEO-$LiClO_4$
L. J. A. Siqueira, M. C. C. Ribeiro. IQ-USP, R. Prof. Lineu Prestes 748, Bl 08 sup. sl 0874, Sao Paulo, SP, Brasil.

08:45 THEORETICAL STUDY OF BTX INTERACTION ON KAOLINITE
E. A. S. Castro, J. B. L. Martins. UnB Instituto de Química-UnB, Q. 604, Asa Norte, Brasília-DF, Brasil, caixa postal: 4478, cep:70919970.

09:00 EXPERIMENTAL AND THEORETICAL STUDIES OF PEROVSKITE $Pb_{1-x}Ca_xTiO_3$ SOLID SOLUTION
S. Lazaro, P. R.Lucena, E. Longo. UFSCar-Liec-DQ, Rodovia Washington Luis, Km 235, Cx Postal: 676, São Carlos, SP, Brazil; Armando Beltrán.UJI; J. A. Varela, J. R. Sambrano. UNESP.

09:15 THEORETICAL MODELLING OF NEW LOW BAND-GAP POLYMER
A. N. S. Costa, J. R. Guimarães, J. G. Amazonas, Jordan Del Nero. UFPA - Rod. Transcoqueiro, Passagem Esportiva n°54.66652-100. Belém, Pará. Brasil

09:30   Invited   THEORETICAL STUDY OF GROWTH OF METAL OXIDE NANOSTRUCTURES
A.Beltrán. UJI. Departament de Ciències Experimentals, 12080, Castellon, España.

10:10   COFFEE-BREAK

Session Chair: Emmanuelle Orhan   (IQ – UNESP)

10:30   Invited   STRUCTURAL AND ELECTRONIC PROPERTIES OF MAGNESIUM CLUSTERS
P. H. Acioli. IF-UnB - Instituto de Física, Universidade de Brasília, Brasília, DF 70919-970, Brazil; J. Jellinek. Chemistry Division, Argonne National Laboratory, Argonne, Illinois 60349, USA.

11:10   PREDICTION OF STATE DIAGRAMS FOR PHOTOACTIVE COMPOUNDS USING AB INITIO METHODS
A. E. H. Machado, T. P. Xavier, S. K. Ferreira, M. F. R. Borges. Laboratório de Fotoquímica, IQ-UFU, P.O. Box 593, Uberlândia, Minas Gerais, Brazil, CEP 38408-100; Bruno Mendes. FAMAT/UFU.

11:25   FULL RELATIVISTIC AND SPIN-ORBIT EFFECTS ON THE $SrTiO_3$ BAND STRUCTURE AND OPTICAL PROPERTIES IN ITS TETRAGONAL PHASE
J. C. Garcia, A. T. Lino, L. M. R. Scolfaro. USP - Departamento de Física dos Materiais e Mecânica, Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970 São Paulo, SP, Brazil; V. N. Freire, G. A. Faria. UFC.

11:40   Invited   CARBON NANOTUBE ADSORBED ON HYDROGENATED Si(001) SURFACES
A. Fazzio, USP, Departamento de Física dos Materiais e Mecânica, Instituo de Física, Universidade de São Paulo, CP 66318, 05315-970 São Paulo, SP, Brazil.

12:25   LUNCH

Wednesday, October 13
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Session Chair: Aguinaldo R. Sousa   (FC – UNESP)

08:00   A THEORETICAL INVESTIGATION ON HgI_2 AND ZnI_2 FUNDAMENTAL PROPERTIES
F. Ayres, W.V.M. Machado, L.V.C. Assali. IFUSP - Departamento de Física dos Materiais e Mecânica, CP 66318, 05315-970, São Paulo, Brazil; J.F. Justo. EPUSP.

08:15	NICKEL COMPLEX IN DIAMOND: A MODEL FOR ELECTRICALLY ACTIVE CENTERS

08:15   NICKEL COMPLEX IN DIAMOND: A MODEL FOR ELECTRICALLY ACTIVE CENTERS
R. Larico, W. V. M. Machado, J. F. Justo, L. V. C. Assali. USP - Departamento de Física dos Materiais, Rua do Matão, Travessa R, 187. CEP 05508-900 Cidade Universitaria, São Paulo - Brasil.

08:30   TWO DIMENSIONAL Si/Ge SUPER-LATTICES ON THE Si(111) SUBSTRATE
R. H. Miwa, T. M. Schmidt, P. Venezuela. UFU - Faculdade de Física, Universidade Federal de Uberlândia, C.P. 593, 38400-902, Uberlândia, MG - Brazil.

08:45   THEORETICAL STUDY OF REACTIONS IN ZEOLITES HZMS-5 AND HY
I. Milas, M.A.C. Nascimento. UFRJ. Cidade Universitaria, CT, Bloco A, Sala 412, Ilha do Fundão, Rio de Janeiro, RJ, Brasil, 21949-900.

09:00   CALCULATED CORE-LEVEL SHIFTS AND ADSORPTION ENERGIES TO INVESTIGATE THE OXIDATION OF THE Si(001) SURFACE
T.M.Schmidt, R.H.Miwa. UFU - Faculdade de Física, Universidade Federal de Uberlândia, Cx. P. 593, 38400-902, Uberlândia, MG, Brazil; J.T.Arantes. USP.

09:15   THE ROLE OF THE NEIGHBOURHOOD IN THE MAGNETIC AND HYPERFINE BEHAVIOUR OF Fe-Mo-Al ALLOYS
R. N. Nogueira, C. G. Schön. EPUSP - Computational Materials Science Lab., Dept. of Metallurgical and Materials Engineering, Escola Politécnica da Universidade de São Paulo, Av. Prof. Mello Moraes, 2463 - CEP 05508-900 São Paulo -SP, Brazil; P. G. Gonzales-Ormeño, H. M. Petrilli. IFUSP.

09:30   Invited   EVOLUTION AND STATE OF THE ART OF THEORETICAL-COMPUTATIONAL-SIMULATIONS FOR THE STUDY AND DESIGN OF NEW MATERIALS
C. Taft, CBPF. Xavier Singaud, 150, Rio de Janeiro, Brazil, CEP 22290-180.

10:10   COFFEE-BREAK

Session Chair: Carlton Taft   (CBPF - RJ)

10:30   3-D RECONSTRUCTION OF FRACTURE SURFACES OF POLYMER MATRIZ COMPOSITES
R. M. Lobo, A.H.P.Andrade, G. Marinucci. IPEN. CCTM, Av. Prof. Lineu Prestes 2242, 05508-900 São Paulo SP; L.R.O. Hein. Unesp.

10:45   STRUCTURE AND DYNAMICS OF IONIC LIQUIDS OF 1-ALKYL-3-METHYLIMIDAZOLIUM CATIONS
M. C. C. Ribeiro. I.Q. - USP Laboratório de Espectroscopia Molecular, Caixa Postal 26077, CEP 05513-970, São Paulo, SP, Brazil; S. M. Urahata. USF Flórida.

11:00   CONFORMATIONAL ANALYSIS AND ELECTRONIC STRUCTURE OF CARBON NITRIDE NANOTUBES
A. C. M. Carvalho, UNICAMP - IQM – DFQ. CP 6154, 13083-970 - Campinas, SP, Brazil. M. C. Santos, UNICAMP - IFGW – DFMC.

11:15   SIMULATING PATTERN FORMATION AND SIZE SEGREGATION OF GRANULAR MATERIALS IN A HELE-SHAW CELL
A. T. Bernardes, E. C. de Souza, H. F. V. de Rezende. UFOP - Departamento de Física, Universidade Federal de Ouro Preto, Campus Morro do Cruzeiro, 35400-000 Ouro Preto-MG, Brazil.

11:30   MOLECULAR DYNAMICS SIMULATIONS ON THERMODYNAMIC PROPERTIES OF SUPERIONIC SYSTEMS
A. Picinin, G.Q. Hai. USP - Instituto de Física de São Carlos, Avenida Trabalhador Sãocarlense, 400. São Carlos, São Paulo, Brazil, CEP 13560-970; M. A. P. Silva, J.P. Rino. UFSCar.

11:45   MAGNETIC PROPERTIES OF METAL-ORGANIC FRAMEWORKS (MOFS) BASED ON DICOPPER(II)-TETRACARBOXYLATE UNITS
A. P. S. Santos. PGMTR - CCEN – UFPE - Av. Prof. Luiz Freire s/n, 50740-901, Recife, PE, Brazil; R. L. Longo, DQF - CCEN - UFPE.

12:00   INTENSE VISIBLE PHOTOLUMINESCENCE OF THE DISORDERED $Ca_xSr_{1-x}WO_4$ COMPOUNDS
V. Longo, P. S. Pizani, F. M. Pontes, E. R. Leite, E. Longo, M. A. Santos. UFSCar Rod. Washington Luiz, Km 235, São Carlos, São Paulo, Brazil,cx postal 676; E. Orhan, J. A. Varela. UNESP; S L. Porto, A. G. Souza,. UFP.

12:15   GEOMETRIC COMPUTATIONAL MODELING EVALUATION OF THE ROLL BONDING PROCESS PORE STRUCTURE OF NUCLEAR FUEL PLATES CONTAINING $(Th,25\%U)O_2$ MICROSPHERES DISPERSED IN STAINLESS STEEL
A. M. F. Lage, S. C. Reis, W. B. Ferraz, CDTN - Centro de Desenvolvimento da Tecnologia Nuclear, Rua Prof. Mário Werneck, s/n, UFMG, Belo Horizonte, Minas Gerais, Brasil, Caixa Postal 941, CEP 30123-970.

12:25   LUNCH

Session Chair: Fabrício Sensato   (FSA – SP)

14:00   Invited   THE ORIGIN OF ROOM TEMPERATURE PHOTOLUMINESCENCE IN DISORDERED COMPOUNDS
E. Orhan. LIEC/UFSCar - Instituto de Química, Universidade Estadual Paulista, 14801-907, Araraquara-SP, Brazil.

14:40   THEORETICAL STUDY OF THE ELECTRONIC STRUCTURE, EFFECTIVE MASSES, AND OPTICAL PROPERTIES OF RUTILE TITANIUM DIOXIDE
C. Persson, KTH - Department of Materials Science and Engineering, Royal Institute of Tecnology (KTH), SE–100 44 Stockholm, Sweden; Moyses Araujo. Uppsala Univ; J. S. de Almeida, R. Ahuja Uppsala; N. Souza Dantas, A. Ferreira da Silva. UFBa; E. F. da Silva Jr, W. M.de Azevedo. UFPE.

14:55   MOLECULAR DYNAMICS SIMULATIONS OF NANOTUBE CARBON PROBE INSIDE OF TOROIDAL CARBON NANOTUBE
A. Maia, J. Del Nero. UFPA - Departamento de Física, Universidade Federal do Pará, 66.075-110 Belém PA BRAZIL.

15:10   Invited   A MOLECULAR DYNAMICS STUDY OF OXYFLUORIDE GLASSES WITH NEUTRAL PARTICLES
R. L. Longo, F. S. L. Borba. DQF-UFPE - Departamento de Química Fundamental - Universidade Federal de Pernambuco - Av. Prof. Luiz Freire, s/n - Cidade Universitária - 50.740-540 - Recife, PE - Brasil.

15:55   COFFEE-BREAK

16:20   POSTER SESSION

INVITED PRESENTATIONS

F-I001   THEORETICAL STUDY OF GROWTH OF METAL OXIDE NANOSTRUCTURES

A.Beltran. UJI. Departament de Ciències Experimentals, 12080, Castellon, España.

One of the challenges in advanced materials is the control of the inorganic nanocrystal morphology. In fact the shape of nanocrystals influences the physical and chemical properties. This is observed for metals, oxides, and semiconductors. Such changes in the physical-chemical properties produce a wide range of electrical, optical, and/or magnetic properties and open a new domain of both fundamental and technological interest. Recently, the synthesis of nanostructures based on metal oxides was demonstrated. Growth of nanoribbons: Two models for the growth of crystalline nanoribbons have been proposed, the vapor-solid (VS) and the vapor-liquid-solid (VLS) processes. Growth of nanocrystals: Any particle system dispersed in a medium and having a certain degree of solubility in it is thermodynamically unstable due to its large interface area. Thus, one way of decreasing the high interfacial energy associated with this large interfacial area is through particle growth, and the mechanism most likely to achieve this reduction is a dissolution-based mechanism such as the Ostwald-ripening. Modern methods of theoretical chemistry are widely recognized and complementary tools to be used, they not only allow interpretations of experimental data to be obtained but also enable new results to be predicted. Therefore, in this work a joint theoretical and experimental study. Calculations based on density functional theory at B3LYP level and periodic slab models have been done.

F-I002   STRUCTURAL AND ELECTRONIC PROPERTIES OF MAGNESIUM CLUSTERS

P. H. Acioli. IF-UnB - Instituto de Física, Universidade de Brasília, Brasília, DF 70919-970, Brazil; J. Jellinek. Chemistry Division, Argonne National Laboratory, Argonne, Illinois 60349, USA

We used gradient-corrected density functional theory to study structural and electronic properties of neutral and anionic magnesium cluster with up to 22 atoms. We performed an analysis of the change in structural motifs as a function of cluster size. We applied our recently developed accurate scheme for conversion of the Kohn-Sham eigenenergies into electron binding energies to compute the electron binding energy spectra as a function of cluster size, charge state, and isomeric form. The computed results are compared with the measured spectra and the true information content of the latter is clarified. A discussion of the size-evolution of electronic properties as an indicator of the size-induced transition to metallicity is given.

F-I003

CARBON NANOTUBE ADSORBED ON HYDROGENATED Si(001) SURFACES

A. FAZZIO, USP, Departamento de Física dos Materiais e Mecânica, Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970 São Paulo.

F-I004 THE ORIGIN OF ROOM TEMPERATURE PHOTOLUMINESCENCE IN DISORDERED COMPOUNDS
E. Orhan. LIEC/UFSCar - Instituto de Química, Universidade Estadual Paulista, 14801-907, Araraquara-SP, Brazil.

First principles quantum mechanical techniques, based on density functional theory (at B3LYP level) were employed to study the electronic structure of symmetric and asymmetric periodic models for a wide range of titanate and tungstate compounds ($BaTiO_3$, $SrTiO_3$, $Ba_{0.5}Sr_{0.5}TiO_3$, $CaWO_4$, $SrWO_4$, $PbWO_4$). Electronic properties are analyzed in the light of the measured photoluminescence properties. The presence of localized electronic levels in the band gap, due to the symmetry break, together with the coexistence of a charge gradient between the network forming clusters would be responsible for the visible photoluminescence of the amorphous compound at room temperature.

F-I005 A MOLECULAR DYNAMICS STUDY OF OXYFLUORIDE GLASSES WITH NEUTRAL PARTICLES
R. L. Longo, F. S. L. Borba. DQF-UFPE - Departamento de Química Fundamental - Universidade Federal de Pernambuco - Av. Prof. Luiz Freire, s/n - Cidade Universitária - 50.740-540 - Recife, PE - Brasil.

Oxyfluoride glasses PbF_2-GeO_2 containing Ag_2O form a thin metallic film after a proper thermal treatment. This film is probably formed from bulk silver nanoparticles. In order to apply these glasses as optical materials, for instance, it is important to comprehend the mechanism for the formation of these nanoparticles, their dynamics (diffusion) and how their form the surface film. Thus, glasses with composition $xPbF_2$-$(100-x)GeO_2$ containing 4 and 15 neutral spherical particles were simulated with the molecular dynamic (MD) method. The interaction potential between the ions has repulsive and electrostatic terms, and a Lennard-Jones potential was used to describe the interactions between the ions and the neutral particles and amongst the neutral particles, where its depth (0.05 - 0.5 eV) and closest proximity (0.10 - 0.2 nm) parameters were varied. The diffusion coefficients were calculated in the 300-1100 K range. The fluorine ions present the largest mobility and the neutral particles have diffusion coefficients at least a hundred times larger than those of the fluorine ions. This can be explained by the weak interaction of these neutral particles and the ionic matrix. It shall then be attempt to study the dynamics of the neutral particles with nanometric sizes.

F-O006   EVOLUTION AND STATE OF THE ART OF THEORETICAL-COMPUTATIONAL-SIMULATIONS FOR THE STUDY AND DESIGN OF NEW MATERIALS
C. Taft, CBPF. Xavier Singaud, 150, Rio de Janeiro, Brazil, CEP 22290-180.

From the fundamentals of quantum chemistry Bohr(1913) to nano-structures, nanotechnology (2004). Evolution and State of the Art of Theoretical-Computational-Simulations for the study and design of new materials: Empirical, Semiempirical, Ab-Initio, Hartree-Fock, Post-Hartree-Fock, Density functional theory, basis functions, LCAO, Band Theory, Pseudopotentials, Molecular Dinamics, Quantum Monte Carlo, (Embedded, Oniom models), Docking Techniques. Study by the group and collaborators of oxides of technological interest (publications and book chapter). MgO, CaO, MnO, EuO, NiO, ZnO, TiO_2, Cu_2O, CuO, $SrTiO_3$, $BaTiO_3$, Fe_3O_4, $LiNbO$, ZrO_2, UO, ? -Al_2O_3, Ti_2O_3, Na_2O. Oxides are of considerable theoretical, experimental and technological multidisciplinary research interest (semiconductors, microelectronics, surfaces, metallurgy, sensors, photoluminescence, corrosion, fuel cells, catalysis, petroleum chemistry). Study and design of surfaces and nano-structures of oxides, doped, modified and their interactions with water, gases and other complexes. Focus on geometry optimization, adsorption, dissociation, bond orders, hydrogen bonding, charge transfer and distribution, molecular energies and orbitals, Fermi levels, density of states, surface reactions, acid-base, cluster and basis size effects, surface planes, doping, impurities, vacancies, steps, kinks, slabs, coverage. Comparison whenever possible between theoretical-computational methods, experiments and technological applications.

F-O001   MAGNETIC MOMENTS AND HYPERFINE FIELDS OF 4d IMPURITIES AND MONOLAYERS IN BCC IRON.

C. Paduani. Fisica, UFSC, SC, Florianopolis, Brazil; J. C. Krause. DCET-URI, Santo Angelo, RS, Brazil.

The full understanding of the mechanism of hyperfine interactions and its relation to the host magnetization still is a challenge in the theoretical research developed in magnetic systems. Although the hyperfine field distribution around an impurity atom can be accurately well described by several current techniques, in more complex magnetic systems as dilute alloys and superstructures or multilayers the situation is not so simple. A question still unsolved is what could be the relation between the atomic local moment and the hyperfine field at the nucleus. Many empirical expressions have been employed that works reasonable in a restrict number of cases and mostly just giving a fair agreement with experimental results. In this work we present first-principles calculations of the magnetic moments and hyperfine fields for 4d isolated impurities and monolayers in bcc iron host. The molecular cluster discrete variational method is used to obtain the electronic structure in spin-polarized calculations in the framework of the local approximation of the density-functional theory. The electronic structure for a structural substitution of a monolayer of 4d atoms in bcc iron is also investigated. In this case the results indicate a stronger hybridization between conduction and valence electrons as well as depleted local moments
as compared with the impurities.

F-O002   MAGNETIC PROPERTIES OF CO_2MnX (X= Al, As) INTERMETALLIC COMPOUNDS AT ZERO AND ELEVATED PRESSURE.

I. Momotaro, J.F. Miguel, V.C. Laudemir. Unesp. Departamento de Física - Av. Emgenheiro Luiz Edmundo Carrijo Coube S/N- Bauru-SP- Brazil - Po BOX 473 - 17033-360; L. Bernardo, A.A. Alexandre, G. Sérgio, C.de A. Adelino, M.A. Marilsa. UNICAMP.

The Co_2MnX (X= Al, As) intermetallic compounds crystallize in L21 structure, cubic Heusler phase. In this work we investigated the magnetic behavior of Co_2MnX (X= Al, As) compounds at zero and elevated pressure. The study was done using Wien 97 code, all electron full potential linearized augmented plane wave method (FPLAPW) with spin polarized energy band calculations based on density functional theory (DFT) within the general gradient approximation (GGA). For these materials our results indicate that the Co and Mn atoms are responsible for most of the magnetic properties. We obtained for the Co_2MnAs compounds the calculated spin magnetic moment at As, Mn and Co sites the values of 0.066 µB, 3.166 µB and 1.342 µB respectively. For Co_2MnAl compound the calculated spin magnetic moments at Al, Mn and Co sites are 0.016 µB , 3.736 µB and 0.279 µB respectively . We also present in this work the total density of states, band energy dispersion curves, total energy per atom as a function of the system volume, as well as the magnetic moment as a function of system lattice parameter. The our knowledge there is no experimental work on Co_2MnAs and the calculated spin magnetic moment of 4.277 µB for Co_2MnAl is in a very good agreement with the experimental results. We also observed the half – metallic and the Slater- Pauling behavior in these materials.

F-O003   TEMPERATURE AND SALT CONCENTRATION EFFECTS ON THE STRUCTURE OF POLYMER ELECTROLYTE PEO-LiClO$_4$

L. J. A. Siqueira, M. C. C. Ribeiro. IQ-USP, R. Prof. Lineu Prestes 748, Bl 08 sup. sl 0874, Sao Paulo, SP, Brasil.

Throughout three decades, Solid Polymer Electrolytes (SPEs) have been investigated as potential candidates for use in secondary lithium batteries and displays due to the ability of poly(ethylene oxide) (PEO) to form free-solvent solutions with alkali salts. Beside PEO-Li halides, PEO-LiClO$_4$ polymer electrolyte is one of most studied SPEs. Several computational simulations, specifically molecular dynamics simulations (MD), of polymer electrolytes have been performed. Good agreement with experimental data has been found, electing the MD as a powerful tool to study not only SPEs but also other materials whose properties can be treated by classical mechanics. In this work, we have reported a molecular dynamics simulation on the PEO-LiClO$_4$ at three salt concentration and two temperature values. Concerning the ion pair formation, decreasing the salt concentration at 373 K gives less formation of ion pairs, because more oxygen atoms of the polymer (Opol.) are available to interact with

the Li$^+$ ion. As a consequence, the number of Opol. neighbor of a Li+ ion has increased. By raising the temperature to 500 K, at a given salt concentration, it was observed an increase in the ion pair formation and a decrease of the Opol. complexation to a Li$^+$. The temperature effect upon the ion pair formation takes place due to entropy effect. When the temperture is raised, the entropy of the polymer increases, what provokes a decrease in the ability of the polymer to solvate the cation.

F-O004   THEORETICAL STUDY OF BTX INTERACTION ON KAOLINITE

E. A. S. Castro, J. B. L. Martins. UnB Instituto de Química-UnB, Q. 604, Asa Norte, Brasília-DF, Brasil, caixa postal: 4478, cep:70919970.

Aluminosilicates appear in different crystal structures having a defined chemical composition and are the main constituent of the earth crust. Zeolites and clay minerals are important examples of aluminosilicates being widely used in technology and industry. Clay minerals are used in paints, cosmetics, ceramics, paper coating, plastics, in recycling water, soil remediation and catalysis. One of most recent and important applications of clay minerals is for environmental remediation due to BTX (benzene, toluene and xylenes) soil contaminant. The simulation methods are a fundamental tool in studying the adsorbing process and to understand the paths related to the interaction. We have used semi-empirical and ab initio methods in order to study the interaction of BTX and kaolinite. The main purpose of this work is to understand the selectivity regarding the BTX constituents and also determine the preferential adsorption sites for these molecules on kaolinite. The $(Al_2Si_2O_9H_4)_3$ cluster model is used for describing kaolinite structure in the 3-21G basis set level and AM1 semi-empirical Hamiltonian. The binding energy, atomic charge population, SCF orbital energies and vibrational frequencies are analyzed.

F-O005   EXPERIMENTAL AND THEORETICAL STUDIES OF PEROVSKITE
$Pb_{1-x}Ca_xTiO_3$ SOLID SOLUTION

S. Lazaro, P. R.Lucena, E. Longo. UFSCar-Liec-DQ, Rodovia Washington Luis, Km 235, Cx Postal: 676, São Carlos, SP, Brazil; Armando Beltrán.UJI; J. A. Varela, J. R. Sambrano. UNESP.

ABO$_3$ perovskites have attracted considerable attention in the last years because they form one of the most important classes of mixed oxides, suitable for various technological applications. On the other hand, significant advances in the structural characterization using DRX were made. The $Pb_{1-x}Ca_xTiO_3$ solid solution has been widely studied due to it´s crystalline phase called pseudocubic. On this solid solution, no adjustment in a tetragonal or cubic phase on the DRX analysis was found. Some ferroelectric and piezoelectric properties of this material are related in the literature but there are doubts about it´s structure. Correlations between theoretical and experimental techniques can bring to light clarification about this structure, therefore periodic ab initio calculations can provide importants informations regarding the electronic and structural properties of solids and interpretation of experimental data. We report a periodic density functional study on selected compositions of $Pb_{1-x}Ca_xTiO_3$. The results are discussed in terms of density of states (DOS), band structure and the structural optimized parameters.

F-O006   THEORETICAL MODELLING OF NEW LOW BAND-GAP POLYMER

A. N. S. Costa, J. R. Guimarães, J. G. Amazonas, Jordan Del Nero. UFPA - Rod. Transcoqueiro, Passagem Esportiva nº54.66652-100. Belém, Pará. Brasil

Conjugated polymers with gap around 1.0 eV have a number of potential advantages over their inorganic counterparts, such as ease of processing, cost of manufacture and greater variety. An emerging area of application for semiconducting polymers is in light emitting diodes (PLEDs), first reported in 1990. Semiempirical calculations levels were performed for new polymers based on thiophene derivatives and obtained a fully optimized geometry. The parameters used in the calculations were the defaults within the MOPAC package, except for the convergence criterion (maximum step size of 0.05 was used instead). For both structures, a planar configuration was assumed as the starting point for the geometry optimization calculations. Based on the above structures, the principal transitions contributing to the optical spectra were identified by INDO/S-CI level. This method was parameterized so as to give the best description of the UV-visible optical transitions, particularly in organic materials. Our results shows that both polymers show a broad, long wavelength absorption consistent with a p-p* transition centred at 968 nm. These trend is also seen clearly which shows the energies of the p-p* transitions in the monomer, dimer, trimer, tetramer and polymer. The data also confirms that by bridging two thiophene moieties with electron-withdrawing groups a significant reduction in the bandgap of the resulting polymer may be achieved compared with polymers based on the 3-alkylthiophenes.

F-O007   PREDICTION OF STATE DIAGRAMS FOR PHOTOACTIVE COMPOUNDS USING AB INITIO METHODS

A. E. H. Machado, T. P. Xavier, S. K. Ferreira, M. F. R. Borges. Laboratório de Fotoquímica, IQ-UFU, P.O. Box 593, Uberlândia, Minas Gerais, Brazil, CEP 38408-100; Bruno Mendes. FAMAT/UFU.

The state diagram of two photoactive metal-phthalocyanines, able to generate singlet oxygen, obtained by the application of two ab initio quantum-mechanical approach (CI-Singles and TD-DFT), is described in this communication, and compared to experimental and PM3-CI data. These compounds have potential application in photodynamic therapy and other technologic fields, being that the knowledge of its electronic structure can be used as a start-point to promote the design of new photo-active molecules with pre-defined characteristics. As expected, TD-DFT gives the best description, with a good agreement in the prediction of singlet (S1) and triplet (T1) energies. The energy diagram justifies well the trend of these molecules in populate the triplet state. The ground state structures were firstly optimized using semi-empirical methods (PM3 and MNDO/d) and then refined using a DFT methodology.

F- O008   FULL RELATIVISTIC AND SPIN-ORBIT EFFECTS ON THE $SrTiO_3$ BAND STRUCTURE AND OPTICAL PROPERTIES IN ITS TETRAGONAL PHASE

J. C. Garcia, A. T. Lino, L. M. R. Scolfaro. USP - Departamento de Física dos Materiais e Mecânica, Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970 São Paulo, SP, Brazil; V. N. Freire, G. A. Faria. UFC.

Strontium titanate ($SrTiO_3$) has a perovskite structure and exhibits a very large dielectric constant. At room temperature it exists in the cubic form, but transforms into the tetragonal structure at temperatures less than 105 K. This transition, being of non-polar character presents litle influence on the $SrTiO_3$ dielectric properties. In this work we perform full-relativistic calculations of the band structure of tetragonal (t-) $SrTiO_3$. Valence- and conduction- band effective masses, as well as some optical properties like complex dielectric function and refractive index of t-$SrTiO_3$ are obtained using the ab initio all electron Full-Potential Linear Augmented Plane Wave (FLAPW) method within the density functional theory and local density approximation. Our aim is to compare the results obtained for the tetragonal $SrTiO_3$ with those of other ab initio calculations for the cubic phase, once the DFT describes well the properties derived from electronic structure at low temperatures.

F-O009   THEORETICAL STUDY OF THE ELECTRONIC STRUCTURE, EFFECTIVE MASSES, AND OPTICAL PROPERTIES OF RUTILE TITANIUM DIOXIDE

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The electronic and optical properties of rutile phase of titanium dioxide TiO_2 are calculated employing a fully relativistic, full-potential linearized augmented plane-wave (FPLAPW) method within the local density approximation (LDA). The LDA is improved by an on-site Coulomb self-interaction correction (SIC) potential as represented in the LDA+U^{SiC} approach. This correction potential is important to include for accurately calculating and predicting electronic and optical properties near the electronic band edges of semiconductors. We present the LDA+U^{SiC} electronic structure $?_j$(k) of the conduction-band minimum and the valence-band maximum. The calculated fundamental band-gap energy E_g agrees very well with photoacoustic spectroscopy measurements. The effective masses are obtained directly from the curvature of the electronic band structure, taken into account the spin-orbit interaction which has a very strong affect on the band curvatures of the valence-band maximum. Both the effective electron m_c and hole m_v masses show strong anisotropic electronic band edges. The effective masses are screened by the electric field from vibrations of the longitudinal optical (LO) phonons, and we therefore calculate also the corresponding polaron masses. The optical properties are calculated within the linear response theory for $?$ k$?$? = 0. We present the anisotropic dielectric function $?$ ($?$) = $?$ $_1$($?$) + $i?$ $_2$($?$), as well as the static $?$ $_1$($?$) and high-frequency $?$ $_1$(0? ? ? ? ? E_g/h) dielectric constants.

F-O010   MOLECULAR DYNAMICS SIMULATIONS OF NANOTUBE CARBON PROBE INSIDE OF TOROIDAL CARBON NANOTUBE

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Molecular motors are essential to the life of a cell. Motor proteins always move along linear tracks in a specific direction, which is dictated by something intrinsic to the protein itself. But how does this happen? How it is possible to create artificially these motors? One clue may be the symmetry of these molecules; where part of a molecule moves in one way and as other part of the molecule moves to opposite direction and this might originate in the physical symmetry necessary to create a variety of new synthetic molecules with properties of a molecular motor. In this kind of model, the direction of the force is entirely the result of directional bias in the diffusional searching process by which the heads find and bind to the next site along the microtubule track. Subsequent conformational changes, possibly involving reversible interactions between the head and the first part of the tail are directional only because the initial binding to the microtubule is directional. In this work, we propose the molecular dynamics simulation for nanotube probe plus toroidal carbon nanotube system that works as molecular motor. The results are based on simulation of 20 ps with step size of 0.001ps without bath relaxation. The temperatures of simulation were 300 k and 500 k. Different sizes of molecular systems will be discussed as well as the efficiency of these materials to produce energy.

F-O011   A THEORETICAL INVESTIGATION ON HgI$_2$ AND ZnI$_2$ FUNDAMENTAL PROPERTIES

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Mercuric iodide (HgI$_2$) in the red tetragonal phase is a semiconductor material with potential applications as room temperature gamma and X-ray radiation detectors. Although its properties has been investigated for more than thirty years, mercuric iodide has drawn increasing attention during the last decade, due some fundamental problems, such as the mechanical instability, low hole mobility, and control over defect concentrations during the material growth, which precludes its widespread use as a detector. In order to investigate some of these fundamental questions, we made a theoretical investigation of the structural, electronic, mechanical, and optical properties of HgI$_2$. From the equilibrium configuration, we obtain the band structure, the density of states, the charge carrier effective masses, and the elastic constants. One of the most interesting properties of HgI$_2$ is the bonding between the iodine planes, which has been suggested to be of the van der Waals type. Our calculations indicated that the binding energy is comparable to the typical London dispersion energy, showing that it has van der Waals behavior. We also obtained the same properties for the ZnI$_2$ crystal in order to compare with that of HgI$_2$, since both materials have the same structure at room temperature.

F-O012   NICKEL COMPLEX IN DIAMOND: A MODEL FOR ELECTRICALLY ACTIVE CENTERS

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Synthetic diamond can be grown by high pressure-high temperature methods, using transition metal alloys as catalysts. However, transition metals may be incorporated in the resulting crystal, generating electrically active centers with absorption bands in the visible spectra. Electron paramagnetic resonance and optical absorption measurements have identified active centers related to isolated Ni and Ni-related complexes involving intrinsic defects or dopants. However, there is considerable controversy about the microscopic structure of those centers. Here we present a theoretical investigation, based on the spin-polarized full-potential linearized augmented plane wave (FP-LAPW) method, to investigate the properties (atomic structures, symmetries, formation and transition energies,
and hyperfine parameters) of nickel-related centers in diamond. Our results are discussed in the context of the microscopic models which have been proposed to explain the active centers in synthetic diamond. Our studies for the substitutional nickel are consistent with the properties of the W8 center. However, the previously proposed microscopic models for the NIRIM centers, based on interstitial nickel impurities, are inconsistent with our results.

F-O013   TWO DIMENSIONAL Si/Ge SUPER-LATTICES ON THE Si(111) SUBSTRATE

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The formation of self-organized atomic arrangements on semiconductor surfaces has been subject of intense experimental and theoretical investigations. In this class of materials the super-lattices (SLs) have attracted a number of studies, not only addressing the fundamental physics, but also due to their potential application on the engineering of nanodevices. In the SLs, different materials are pilled up in the growth direction forming a three dimensional hybrid structure. However, ver recently, Kawamura et al. [Phys. Rev. Lett. vol. 91, 96102 (2003)] obtained two dimensional (2D) nanowires and nanorings of Si/Ge on the Si(111) substrate, by using Bi as a surfactant element. In fact, this structure can be considered as a 2D SL of Si/Ge. In this work, we have performed an ab initio total energy investigation of the 2D Si/Ge super-lattices on the Si(111) surface. Initially we examined the energetic stability of the Bi adatoms at the surface topmost layers, since Bi acts as a surfactant. We find that the Bi-trimers on the T4 sites of the Si and Ge (top) monolayers represents the energetically most stable atomic configuration. The equilibrium geometry has been detailed, where we find that the Bi-trimers on the Ge monolayer is slightly higher, by 0.10 angs., compared with the Si monolayer. Concerning the electronic structure, we find that the LUMO state lies at the Si monolayer of the SL.

F-O014   THEORETICAL STUDY OF REACTIONS IN ZEOLITES HZMS-5 AND HY

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Petrochemical processes have been extensively studied with theoretical methodologies over the last decade. The search for an environmentally-friendly, non-corrosive, and efficient solid acid catalyst has been the main objective of such studies. Zeolites and zeolite-based catalysts have been the most commonly studied candidates, because of their high surface area and well-defined structure. The overall mechanism of hydrocarbon conversion in zeolites is very complex and it still remains unclear. However, some recent theoretical studies unvieled the general aspects of some of the individual reactions. In this work, we have compared the intermediates and transitions states of the dehydrogenation and cracking reactions in zeolites HY and HZMS-5. The ring clusters we used are able to mirror not only the acid site strucutures, but also the specific cavity environments inside a zeolite framework. All stationary states were obtained without imposing any restrictions on the geometrty and all the calculations were done using the DFT methodology. The calculations have provided interesting information about the mechanisms of the two reaction and have given further insights on how to increase the activity and better the selectivity of the catalysts.

F-O015   CALCULATED CORE-LEVEL SHIFTS AND ADSORPTION ENERGIES TO INVESTIGATE THE OXIDATION OF THE Si(001) SURFACE

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Using first-principles full core potential calculations we investigate the oxygen adsorption processes on the Si(001) surface. Our optimized total energy calculations yield four energetically stable configurations for the sub-oxide Si{1+}, three configurations for Si{2+} and two configurations for Si{3+} components. Our computed initial state Si 2p core-level shifts for the most stable configuration, of each Si{n+} specie, gives -0.96, -1.89 and -2.28 eV for n=1, 2 and 3, respectively. These results are in good agreement with high-resolution photoemission spectra, which allows the determination of the structural model of each Si{n+} specie. We also observed a connection between the adsorption energies of the structural models and the measured intensity ratios of each sub-oxide component. Our calculated adsorption energies indicate an energetic preference to the formation of the Si{2+} structure followed by the Si{1+} and the Si{3+} structures, in agreement with experimental intensities for low O_2 dose results.

F-O016   THE ROLE OF THE NEIGHBOURHOOD IN THE MAGNETIC AND HYPERFINE BEHAVIOUR OF Fe-Mo-Al ALLOYS

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Fe-Al alloys have attracted much attention due to its challenging magnetic properties as well as possible technological applications and form an interesting class of intermetallic materials which are possible candidates for substitution of stainless steel in structural applications at moderate to high temperatures. In this work, we analyse the influence of the neighbourhood on the magnetic and hyperfine behaviour at Fe sites in bcc-based Fe-Al, Fe-Mo and Fe-Al-Mo alloys. Theoretical ab initio calculations were performed in the framework of density functional theory using the Full Potential – Linear Augmented Plane Wave method as embodied in the WIEN97 code. The analysis is made through local magnetic moments considering the distribution of the first coordination shell of the Fe atoms. For the magnetic moments, we find that it is nearly independent of the composition in Fe-Mo binary. Although the magnetic behaviour of Fe-Al alloys is a very complex and controversial subject, our results clearly shows that an increase in the number of Al nearest neighbours leads to a decrease or even suppress of the local moment at Fe sites. The ternary bcc-based Fe-Mo-Al alloys present no correlation between magnetism and nearest neighbourhood composition. Nevertheless, as expected, the Fe moments are larger when its first neighbouring shell has more Mo atoms and smaller when it has more Al atoms. For the hyperfine fields, we compare our results with an empirical model.

F-O017   3-D RECONSTRUCTION OF FRACTURE SURFACES OF POLYMER MATRIZ COMPOSITES

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Analyses of the fracture surfaces on the basis of 2-D images is restricted to the understanding of qualitative features of the fracture. This limitation opens way for the possibility of considering more information associated to the 3-D morphology of fracture surfaces. In fiber reinforced composites, the matrix/fiber interface strongly influences its physical and mechanical properties, and even so many methods to measure the shear strength have been developed and applied to different matrices, for different types of fiber, few of them take into account the distribution of fiber pullout lengths in the fracture surface. Measurement of these lengths in relation to the matrix fracture surface, taking as planar reference, is applicable only for matrices of high stiffness, with a low fiber volume fraction, as in the ceramic matrices. For polymeric or metallic matrices, the fracture surface is usually not smooth, what leads to a different approach to evaluate the height distribution of breaking fibers. Techniques of image processing and analysis can contribute for the quantitative fractography. By using a software associated with the image processing based on microscopy the 3-D reconstruction of fracture surfaces is possible, that is more effective for rough regions as the formed ones by dimples. The goal of this work is to study the 3-D reconstruction of fracture surfaces of polymeric matrix composite materials reinforced by carbon fibers.

F-O018   STRUCTURE AND DYNAMICS OF IONIC LIQUIDS OF 1-ALKYL-3-METHYLIMIDAZOLIUM CATIONS

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Molecular dynamics (MD) simulations of room temperature molten salts (ionic liquids) containing imidazolium cations have been performed. Ten different systems were simulated by using united atom force fields, in which the anion size (F^-, Cl^-, Br^-, and PF_6^-) and the length of the alkyl chain of 1-alkyl-3-methylimidazolium cations (1-methyl-, 1-ethyl-, 1-butyl-, and 1-octyl-) were systematically varied. Resulting equilibrium structures account for the observed features of experimental static structure factors when available. By increasing the length of the alkyl chain, nearest-neighbor anions around a given cation are pushed away from the volume occupied by the flexible alkyl chain. Partial structure factors of 1-butyl- and 1-octyl- derivatives display a peak at wave-vector smaller than the main peak, indicating the occurrence of an intermediate range order in these ionic liquids due to the presence of long alkyl chains. Despite of large mass and size of imidazolium cations, they exhibit larger mean square displacement than anions due to anisotropy in the cation motion. Vibrational density of states is compared with experimental optical Kerr effect spectra recently reported in the literature. Time correlation functions of reorientation and of dihedral angles of the alkyl chains are discussed, the latter decaying much faster than the former. A comparative physical picture of time scales for distinct dynamical processes in ionic liquids is provided.

F-O019 CONFORMATIONAL ANALYSIS AND ELECTRONIC STRUCTURE OF CARBON NITRIDE NANOTUBES

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Carbon nanotubes (CNT) are a new class of materials discovered recently. They are one-dimensional systems that are built from a graphene sheet rolled into a cylindrical shape. It has been predicted that the electronic structure of CNT´s depends upon the rolling-up direction. The electronic structure of CNT´s could be further manipulated through a convenient doping process – the substitution of carbon atoms by other chemical species, such as nitrogen – or even through the introduction of topological defects in the hexagonal carbon network. In this work we investigated theoretically the conformation and electronic structure of pure and nitrogen-doped CNT´s. Techniques used were Parametric Method 3 (PM3), a Hartree-Fock based methods, and ab intio methods derived from the Density Functional Theory. The conformation analysis performed on the optimized geometries showed that zig-zag nanotubes presented a uniform structure of chemical bonds while armchair nanotubes presented a distorted geometry along the tube axis. Our theoretical simulations of doping process of CNT´s led us to conclude that bamboo shape of carbon-nitride nanotube is due to the defects induced by the incorporation of nitrogen. Modifications on electronic structure due to the substitution of carbon atoms by nitrogen ones in the hexagonal network were also analyzed. This work was supported by CNPq. Computational support from CENAPAD is acknowledged.

F-O020 SIMULATING PATTERN FORMATION AND SIZE SEGREGATION OF GRANULAR MATERIALS IN A HELE-SHAW CELL

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Granular materials can be thought as an intermediate state of matter, between fluids and solids. Under vibration, they can flow as a fluid, but also agglomerate if the frequency is low enough. They are formed by particles which are in contact and only compression forces are present. Granular materials are used in many different fields and applications, from cement to food industry, from chemical/pharmaceutical to metallurgy and solid fuel production. So, the understanding of their behavior is extremely important. It is well known that the analytical treatment of such class of materials is complicated. In general, only limit solutions can be obtained, and only special cases can be studied by this approach. Consequently, computer simulations are an important tool in the study of many phenomena present in this class of materials. One experiment where segregation and pattern formation is observed, is the injection of mono disperse particles in a medium previously filled by particles of different size. This phenomenon is similar to fluid invasion, where viscous fingering is formed. However, such non linear phenomenon is not well understood in the case of grains. In this work, we propose a purely geometrical model which simulates the invasion of grains in grains of different sizes occurring in a Hele-Shaw cell experiment. We show that the pattern formation and segregation depends only on the size of the particles, supporting previous experiments.

F-O021 MOLECULAR DYNAMICS SIMULATIONS ON THERMODYNAMIC PROPERTIES OF SUPERIONIC SYSTEMS

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Molecular dynamics simulation was performed in order to study superionic solids. Our interest is to bring a contribution to the understanding of high ionic conductivity, through the observation of the diffusion processes of ions on material bulk. Based on classical MD simulations, we performed structural and dynamical analysis of superionic solid solutions for the system $Cd_xPb_{1-x}F_2$. We observed that the difusion of fluor atoms in these materials increases after a phase transition, the so-called ionic-superionic transition, which occurs at temperatures, Tt, well below the melting temperature, Tm, while the positions of lead and cadmium atoms are restrict to the vibrational motion on the regular sites of the cubic lattice.

The technique of molecular dynamics allows the access to properties many times of dificult experimental observation, as the detailed trajectory of the moving ions. On the superionic phase, it is possible to observe the existence of prefered sites for the diffusive fluorine atoms to move. Due to a

correlation with the \'rigid\' cationic sublattice (i.e. T < Tm), the fluor atoms move from one site to another by jump motions. The high ionic conduction of these kinds of material allows numerous technological aplications. $Cd_xPb_{1-x}F_2$ solid solutions are characterized as electrolytes of great importance in the electric microbatteries technologies. The simulations were performed using the Buckingham pair potential.

F-O022   MAGNETIC PROPERTIES OF METAL-ORGANIC FRAMEWORKS (MOFS) BASED ON DICOPPER(II)-TETRACARBOXYLATE UNITS

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Metal-Organic Frameworks (MOFs) are crystalline porous materials that are hybrids formed by metal(-oxide) clusters (Zn_4O, Cu_2) connected by rigid organic bridges (di or tri-benzene-carboxylates). These materials can be used for gas storage, sensors, catalysts, and when the metal ions have unpaired spins, as magnetic materials. The dicopper connected by four carboxylates ($HCOO^-$) and saturated with water models the building units of the $[Cu_3(TMA)_2(H_2O)_3]n$ nanoporous material, where TMA is benzene-1,3,5-tricarboxylate. The model system $[Cu_2(OOCH)_4(H_2O)_2]$ has been simulated by Hartree-Fock (HF) and hybrid DFT (B3LYP and PBE1PBE) methods for the singlet and triplet spin multiplicity states. Comparing the singlet (S) and the triplet (T) state optimized geometries the $Cu-OH_2$ bond distances decrease from S to T and the structure becomes asymmetric. However, this asymmetry has different trends when the functional changes from B3LYP to PBE1PBE, namely, the Cu-OOCH bonds decrease for the former and increase for the latter. Also, the S – T energy differences are 137.4 and 176.8 kJ/mol for B3LYP and PBE1PBE, respectively. These energies are quite large, and a more appropriate functional B3LYP* shall be used to calculate them. Also, the effects on the S-T separation of other ligands such as NH_3 and PH_3, as well as, the $Cu-OH_2$ distances shall be investigated.

F-O023   INTENSE VISIBLE PHOTOLUMINESCENCE OF THE DISORDERED
$Ca_xSr_{1-x}WO_4$ COMPOUNDS

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Visible photoluminescence (PL) is observed at room temperature for the CSW ($Ca_xSr_{1-x}WO_4$, with x = 0.0, 0.2, 0.4, 0.6, 0.8 and 1.0) powders in their disordered and crystalline forms. A study of the PL behavior of CSW powders in function of x and of the disorder rate is performed through experimental and theorical studies. The CSW compounds have been synthesized by the polymeric precursors method, their geometry has been confirmed by X-ray diffraction data and corresponding photoluminescence properties have been measured using a blue-green excitation line (488 nm). The photoluminescence intensifies with the increasing degree of disorder in CSW compounds. From the theoretical side, first principles quantum mechanical techniques, based on density functional theory at B3LYP level, have been employed to study the electronic structure of two periodic models, representing both the crystalline and disordered powers. The calculations indicate that the symmetry break on going from crystalline to disordered models creates localized electronic levels above the valence band and that a negative charge transfer process takes place from $[WO_3]$ cluster to $[WO_4]$ cluster. The conjunction of both effects seems to be responsible for the photoluminescence of the disordered CSW compounds.

F-O024   GEOMETRIC COMPUTATIONAL MODELING EVALUATION OF THE ROLL BONDING PROCESS PORE STRUCTURE OF NUCLEAR FUEL PLATES CONTAINING (Th,25%U)O$_2$ MICROSPHERES DISPERSED IN STAINLESS STEEL

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In this work, the evaluation of the resulting pore structure of a nuclear fuel plates manufacturing process is presented, using a geometrical computational modeling scheme. These fuel plates are obtained from a stainless steel picture-frame roll bonding method, containing compacts of (Th, 25%U)O$_2$ microspheres dispersed in a stainless steel powder. The sol-gel process obtained microspheres were previously dried, reduced and sinterized for two hours at a temperature of 1700 ^{o}C, under a hydrogen atmosphere, reaching a density of about 100% of the theoretical density, a 300 micrometer average diameter and a 40 N/microsphere fracture resistance. The microstrutures of the longitudinal cut fuel plates were analyzed for hot rolling resulting typical pore microstructure characterization using a CDTN proprietary developed model that simulates this process. The implemented rules of that model were applied over a sphere surface points and the geometrical shapes obtained matched the pore structure previously verified. The model was implemented using DELPHI and the geometrical shapes viewed using AUTOCAD. We expect that the results of this work could be used to reach pore structure matching nuclear fuel plates design specifications.

F-P001   SILVER DIFFUSION AND CLUSTERING IN OXYFLUORIDE GLASSES

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Oxyfluoride glasses have good optical properties similar to fluoride glasses and high chemical stability similar to oxide glasses. In the GeO_2–PbF_2 glass matrix doped with low quantities of Al_2O_3 and Ag_2O a silver thin film was observed after the annealing and thermal treatments. A molecular dynamics (MD) study has been performed to propose a microscopic mechanism for this phenomenon. We have used the NPT ensemble in the program DLPOLY with a combination of the Born-Mayer-Huggins model for the ions and the Lennard-Jones pair potential for the silver atoms interactions. The results showed a good agreement between the calculated and observed glass transition and melting temperatures, thus suggesting that the MD simulations are converged and the potential describes the system properly. Also, a high ionic conductivity of the silver ions similar that of fluoride ions were calculated and silver atom clustering was observed near the annealing temperature. Understanding and controlling the structure of these glasses is relevant in the development of new materials that can be applied in solid state batteries or in fiber optics.

F-P002   INDIRECT DETERMINATION OF THE ELECTRONIC STRUCTURE OF $Pb_{1-x}La_xTiO_3$

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It is well stablished that materials possessing $ATiO_3$ structure can present eletric properties. In addition, one of the most important ferroelectric materials is the lead lanthanum titanate (PLT). This compound have been extensively studied due to its potencial application in dynamic random access memories (DRAM), uncooled infrared detectors and electro-optic devices. However, these properties are strongly dependent on the amount of La added to the lead titanate structure (PT). This work presents the study of the structure electronic of $Pb_{1-x}La_xTiO_3$ with x = 0, 0.05, 0.10, 0.15, 0.20, 0.25 and 0.30 of the La. In this study, experimental data from Rietveld refinements were used as parametres in the periodic calculations using the CRYSTAL98 software. This was accomplished applying the distortion effect of the lattice caused by the La atom. This methodology, indirect determination of the electronic structure, was develop, since it was not found a base set for the La atom.

F-P003 PHENOMENOLOGICAL EVALUATION OF Er^{3+} DOPED GLASSES FOR ULTRAFAST FIBER AMPLIFIER APPLICATIONS

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In this work we have carried out a phenomenological study of the optical emission in Er doped fiber glass materials which can be used for fiber amplifier applications. Modelocked femtosecond lasers have nowadays found their way into a widespread variety of both scientific and industrial applications. In contrast to bulk crystals femtosecond lasers, erbium-fiber lasers do not require large dispersion-compensating schemes, due to their soliton regime that permits the stable generation of picojoule femtosecond pulses at low and adjustable repetition rates. As another advantage, Er fiber lasers can be diode pumped. Because erbium lasers can produce femtosecond pulses in the wavelength range 1530–1610 nm, frequency doubling can be used to reach 765–805 nm. The use of the diode at 970 nm also allows building such an erbium laser without a high voltage supply. To describe the diode pump laser process, a theoretical model based in a coupled system of differential rate equations was developed. This system of equations is numerically solved and the used approaches and results are discussed. The results corroborates that here are the most important factors in selecting the right fiber material: it must have high fluorescence emission intensity at the desired wavelength; the stimulated emission cross-section should be as large as possible in order to realize high gain; the nonradiative decay due to concentration quenching can greatly decrease the pump absorption efficiency.

F-P004 INVESTIGATION OF THE MAGNETIC HYPERFINE FIELD AT ^{140}Ce ON Nd SITES IN NdAg COMPOUND

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Perturbed gamma-gamma angular correlation (PAC) technique was used to measure the magnetic hyperfine field (MHF) at Nd site in the intermetallic compound NdAg using the 140La-140Ce nuclear probe. A major and well-defined magnetic interaction is observed at 140Ce substituting for Nd sites in NdAg below 22K, corresponding to a ferromagnetic ordering of Nd moments. The results will be interpreted with the aid of first principles eletronic structure calculations.

F-P005 PLASMIC - SOFTWARE FOR CHARACTERIZATION OF CVD DIAMOND FILMS
DEPOSITED BY MICROWAVE PLASMA REACTOR

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PLASMIC is a dedicated software developed to determine all of the diamond film deposit characterizations using the microwave plasma assisted technique. One main objective of this program is to obtain, calculate and present data so as to gather all of the available daily report information on the CVD diamond deposition process in a coherent form.   The software runs in any compatible PC computer. In the general input block of the program, the following data are entered: sample name; sample material; sample shape and dimensions; sample mass before and after deposition of CVD diamond film; gas mixture used; gas flux; environmental and deposition temperatures; deposition time and the internal pressure of the microwave plasma reactor; CVD diamond peak positions along with unstressed peak displacement; coefficients of the sample and film thermal expansion, and the Young biaxial module of the film. In the output block, once having processed all previous data, the program displays: the required power by the microwave reactor; the power density; the useful mass and character of the deposited diamond; the average thickness of the diamond film deposited on the sample; the rate of film deposition in micra/h and in (micrograms/h)/cm^2; the volume of deposited film; the displacement of the Raman spreading peak; the total stress (both thermal and intrinsic); and the classification of the stress   (if it is by compression, null or traction). The software also saves a retrievable file containing the results of the input data. A hardcopy of it can be printed showing all the input/output data information. The software is friendly and requires minimum hardware configuration to furnish all of the characterization data of a deposited CVD diamond film.

F-P006 SOFTWARE FOR DETERMINATION OF THICKNESS, TOTAL STRESS, THERMAL AND INTRINSIC AND THE USEFUL MASS OF CVD DIAMOND FILMS DEPOSITED BY HOT FILAMENT REACTOR

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HOTFILA is a dedicated software designed to help researchers and other people engaged in activities of developing data before and after the essays of CVD Diamond deposition on the square/rectangular, circular or triangular substrate surface samples in order to provide quick and dependable calculations involving parameters related to CVD diamond film deposited by hot filament reactor. The software runs in any compatible PC computer under Windows platform, describes all the main parameters of the sample as: the basic material being analyzed, its geometrical dimensions, densities, thermal expansion coefficient, peak values and Raman scattering displacement. It also allows to describe the mixture components, mainly formed of hydrogen, methane and other gas so as to define a better quality of the CVD diamond and its volume percentage, the gas flux, the deposition time, the reactor internal pressure and the CVD diamond deposition temperature. Equally, the software calculates the film deposition rate, the deposited mass by area/hour, the total and intrinsic stress, whether be it by compression, null or by traction. All of the results of the calculations are displayed in an organized form and automatically saved in a *.txt format file.

F-P007 THEORETICAL ANALYSIS BASED ON SOLUTION OF RATE EQUATIONS OF TM:YLF BLUE UPCONVERSION LASER PUMPED BY HIGH INTENSITY INFRARED LASERS

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The development of compact blue lasers based on up-conversion processes in Thulium (3+) doped solids, has generated considerable interest among laser scientists due the important applications of this wavelength in memory storage devices and medical surgery and diagnostics, among others. In this work we have studied $YLiF_4$ (YLF) crystals pure and doped with 1mol% Tm (3+) concentration and doped with 100 micro-mol of O (2-). Pure YLF samples were grown by zone refine method, and doped samples were grown by Czochralski technique. The samples were oriented, cut and polished to 2mm thickness. Every sample was irradiated with electron beam (1.5 MeV, 0.7 mA, 2.8 kGy/s) during 18 seconds at room temperature, and also with a Ti:Sapphire CPA system (coherent Mira-Seed-R plus Quantronix Odin) producing pulses centered at 830nm with 750mJ of energy and 60fs of pulse duration (FWHM), with a repetition rate of 1kHz during the same 18 seconds at room temperature. Both kinds of irradiation produced photochromic damages (pure YLF and YLF:Tm) and color centers (YLF:O) that have absorption bands in UV and visible range. From a phenomenological model we studied the interaction between the created defects and thulium ions, and their influence in photobleaching and photodarkening behavior, that are detrimental start-up effects in blue lasers based in thulium transitions pumped by high intensity lasers. Finally blue YLF:Tm laser output power is computed using a rate equation analysis.

F-P008 FULL-RELATIVISTIC CALCULATIONS OF THE OPTICAL PROPERTIES AND CARRIER EFFECTIVE MASSES OF ZrO_2 MONOCLINIC, TETRAGONAL AND CUBIC

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Zirconia (ZrO_2) is one of the most important high-dielectric constant material for silicon dioxide replacement due do the shrinkage of the gate oxide thickness to less than 10 nm. Recently, it was shown the possibility of the existence of the monoclinic, tetragonal and cubic phases in ZrO_2 films deposited on fused silica due to annealing at different temperatures. The crystalline structure of the gate oxide after annealing processes is a key issue for the device operation. Some results based on first principle calculations of the structural and optical properties of ZrO_2 were already published, but without taking into account relativistic effects nor explicitly presenting values for the ZrO_2 carrier effective masses, which are fundamental to the modeling of tunneling currents through floating gate memory devices with ZrO_2 as tunneling oxide, for example. In this work, we present state of the art full-relativistic calculations of the structural and optical properties, as well as the carrier effective masses of ZrO_2 in the monoclinic, tetragonal and cubic phases. We obtain the conduction- and valence-band effective masses in the most important symmetry directions, which are shown to be highly anisotropic. Relativistic effects are demonstrated to be important for a better evaluation of the effective mass values and the detailed structure of the frequency dependent dielectric function.

F-P009   EFFECT OF CATIONS CONFORMATIONS IN THE CONDENSED PHASE OF IONIC LIQUIDS

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Ionic liquids are considered as environmentally friendly. This fact has origin in the possibility of these liquids can substitute volatile organic solvents, because they have low vapor pressures and usually their ability as catalysts. In addition, ionic liquids have chemical and thermal stability, nonflammability, high ionic conductivity, and a wide electrochemical potential window. Conformational analysis was performed in BMI+ cation (1-n-butyl-3-methylimidazolium) from the one initial conformation optimized with first principles methods. From this analysis were selected three stable conformations of the cation's n-butyl chain. Monte Carlo (MC) simulations were performed utilizing each one these conformations with the anions Cl^- and BF_4^-. It was verified that the flexibility of the n-butyl chain is probably the main reason for the disorder of these salts leading to a liquid state.

F-P010   FIRST PRINCIPLES STUDY OF $YNiO_3$

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The perovskites structures $RniO_3$ (Nd, Pr, Eu, Y) present a rich variety of electronic, magnetic and structural properties. In particular, these materials suffer a metal-insulator transition as a function of the temperature and the ionic radius of the rare earth. The insulator phase, at low temperatures, shows na atiferromagnetic order with an unusual propagation vector ($\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$). The metallic phase, at high temperatures, is paramagnetic. Depending on the radius of the rare earth, these systems can also present an intermediate paramagnetic insulating phase. The theoretical treatment of these materials requires the use of models that take into account the strong coulombic interaction among the valence electrons. These models depend of many empirical parameters or previous physical assumptions. It would be interesting if one could estimate the values of these parameters with the accurate first principles methods available today. One of these first principles methods is based on the Hartree-Fock (HF) theory. Although the HF theory completely neglects the electronic correlation is capable to give accurate results for one-electron quantities as electronic densities of states, bandwidths. In this work, we report the application of the unrestricted Hartree-Fock theory to the problem of the perovskite $YNiO_3$. The paramagnetic and antiferromagnetic phases have been studied. The HFcalculations correctly predict a metallic state for the antiferromagnetic phase.

F-P011   STUDY OF HYDROGEN ABSORPTION BY MAGNESIUM CLUSTERS

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By means of the density functional theory in a generalized gradient approximation (GGA), we studied the behavior of magnesium clusters as hydrogen reservoirs. Starting from previous results regarding Mgn clusters, new structures of MgnHm were built through the constant addition of hydrogen of both, atomic and molecular, forms. The calculations of the binding energy between the atomic/molecular hydrogen show that, initially, the atomic hydrogen-magnesium binding energy is stronger than the molecular hydrogen-magnesium energy. However, as the number of hydrogens increase, molecular hydrogen start to occur on the MgnHm clusters.

F-P012   COMPUTATIONAL SIMULATION OF ASPHALTENE AGGREGATES

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The molecular mechanics and molecular dynamics methods were used to explore the complex behavior of asphaltene aggregates. Conformational search of the monomers and dimers was realized and the molecular conformation of minimum energy obtained showed that the aggregate have nearly planar aromatic regions forming stacks in the solid state in order to maximize the attractive intermolecular C…C interactions. The presence of alkyl and cycloalkyl groups in the edges of the model asphaltene molecule introduces additional contributions to the molecular recognition process because may perturb the interactions between the aromatic rings if their spatial conformation is such that steric hindrance is produced when the molecules approach each other. The dimmer is more stable in 80 kcal/mol than two monomers. Simulations of trimers and tetramers on the periodic conditions and calculations of thermophysical properties are being realized with the goal of understanding how specific interactions can control the phase behavior and phase separation phenomena of these complex systems.

F-P013   ONIOM CCSD/RHF STUDY OF THE INTERACTION OF SMALL MOLECULES ON ZnO SURFACES

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The interaction of CO, CO_2, H_2O and NH_3 with oxide surfaces and in particular with the ZnO surfaces show several applications, mainly for the catalysis. Analysis of interaction of small molecules over ZnO surface using the cluster model approach within the Oniom three layers methodology offers an opportunity to probe the validity of this methodology, as well as to the understanding of electronic and structural properties of adsorption. We have used the Oniom method with three layers of theory in order to study the interaction of CO, H_2, CO_2, H_2O and NH_3 small molecules and the dissociation of H_2O and H_2 on ZnO (1010) surfaces. The large cluster model $(ZnO)_{348}$ was used for the surface simulation. The 3-21G basis set was used at RHF level and the correlation CCSD method. The layers are divided into: the high layer at CCSD level, the medium layer at RHF level and the low level layer using the universal UFF force field method. We have taken the full optimization of geometry parameters. The orbital energies, binding energy of adsorbed molecules, Mulliken and ChelpG charge values and geometry parameters were analyzed and compared to the available experimental and theoretical data.

F-P014 THEORETICAL STUDY OF THE ELECTRONIC STRUTURE, CHEMICAL BONDING AND SURFACE EFFECTS OF SLABS OF $KNbO_3$ IN THE PARAELECTRIC CUBIC PHASE
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The electronic energy band structure, density of states (DOS) and charge density of bulk and slabs of $KNbO_3$ in the face centred cubic cell (paraelectric phase), has been theoretically investigated by means of a DFT based methodology. The calculations were performed for slabs of seven monolayers thick with two relaxed terminated surfaces (NbO_2 and KO) and the results compared. The goal is to compare slabs of a few monolayers thick (around 12 angstroms), with the bulk behaviour ant the role of the of the surface termination in this behaviour. The methodology employed is compared with other calculations reported. The bulk presents a fermi level of 1.44 eV and a band gap of 2.96 eV. From the total DOS obtained from the calculations is found that there is a significant hybridization between Nb d and O p states in the compound. Analisys of the nature of the chemical bond indicates that the Nb-O bonds have a partial covalent character, whereas the K-O bonds are predominantly ionic. It is observed a small difference in the surface energy obtained for both slabs. The relaxed optimal positions are most proeminent for Nb and K at the first layers. The surface dipoles points toward the bulk in both terminations. The electronic structure shows a splitting of the lowest conduction bands for the NbO_2 terminated surface. The results yield band structures in agreement with previous theoretical studies, with a indirect band gap. In this aspect, bulk and slab present a behaviour quite similar.

F-P015 SIMULATION OF SPATIAL PATTERNS IN ELECTROHEMICAL PREPARED PbO_2
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Disorder to order transitions driven by self-organization of the dissipative structures presents a great relevance for materials preparation. Unexpected spatial organization in micro- or nano-scale could be achieved simply by controlling dynamic features of the nonlinear systems operating far from equilibrium. Since electrochemical kinetics is inherently nonlinear, and electrochemical experiments are usually performed far from equilibrium, several self-organizing electrochemical systems could be found. However, the direct observation of spatial patterns in electrochemical prepared material is rarely reported. In the present work, a kinetic model to explain the spatial patterns observed in the morphology of PbO_2 deposits on carbon is proposed. The model is closely related with Brusselator scheme used to explain the formation of classical Turing patterns. The integration of the reaction-diffusion equations trough finite differences and Monte Carlo methods are explored. For certain values of the model parameters, the stability of numerical methods requires time and/or space steps which are impracticably small. Nevertheless, under proper initial conditions, the methods work and several spatial patterns were obtained. In particular, a parallel line deposition of the PbO_2, observed by Shen and Wei was simulated.

F-P016   THEORETICAL AND EXPERIMENTAL PROPERTIES OF XANTHONE DERIVATIVES

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The xanthones derivatives are interesting because they could act as inhibitors of enzymes, anti-inflammatory, anti-oxidant, anti-thrombotic, antiviral, besides showing neuropharmacological effects. Very many different routes to synthesize xanthones are known, including general classic synthetic approaches that involve the connection of two aryl fragments to form the internal pyranone ring, and others as cyclodehydration of benzophenones and cycliacylation of benzoic acids. Natural xanthones have been isolated from plant species (eg. Clusiaceae, Gentianaceae, Hipericaceae family) found, especially, in tropical areas. In this work, the xantones were obtained by synthetic procedure and were isolated from Kielmeyera variabilis Mart. (Clusiaceae).

Sophisticated calculation methodology based on density functional theory (DFT-B3LYP/6-31G) was utilized for the simulation of systematic geometry optimizations. To obtain a realistic description of the electronic transitions, it was necessary to use methods specially developed to handle these aspects, and we have adopted the INDO/S-CI (intermediate neglect of differential overlap / spectroscopic - configuration interaction) method in this investigation. We have carried out INDO/S-CI calculations using on the average 200 configurations with the geometries obtained from B3LYP/6-31G calculations. As an example of a new effect predicted to occur in xanthone we present results for a specific family of these compounds.

F-P017   A NEW METHOD TO DESIGN BASIS SET FOR DESCRIBING ATOMIC CENTERS TO BE USED IN MOLECULAR OR PERIODIC CALCULATIONS

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One of the common sources of problems with periodic calculations is the appropriate choice of basis sets. The basis sets used for solids are Bloch functions modulated over the infinite lattice. Any attempt to use large uncontracted molecular or atomic basis sets with very diffuse functions result in wasting of computational recourses. In this sense, the dense packed nature of many crystalline structures give rise to a large overlap between the basis function, and a quasi-linear dependence can occur. In order to address this problem we have developed a simple method based on density matrix theory to analyze, model and contract basis set to be used along with pseudopotential in periodic and molecular calculation. This formulation leads to a continuous representation of the density matrices as functions of a generator coordinate, and to the possibility of plotting either the continuous or discrete density matrices as functions of the exponents of primitive Gaussian basis functions. The procedure was employed to design Gaussian basis sets for Sn and O atoms to be used in the investigation of the electronic and structural properties of bulk SnO_2. Compact effective pseudopotential (CEP) was used to represent the core electrons of each atom. The calculations predict a band gap of 3.4 eV, which is located at the gamma-point of the Brillouin Zone, in agreement with experimental results.

F-P018   ANALYSIS OF STRUCTURAL, ELECTRONIC AND PHYSICAL-CHEMISTRY PROPERTIES OF FLUORENE-BASED MONOMERS USING QUANTUM-CHEMICAL METHODS

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The luminescent properties of conjugated polymers have stimulated many experimental and theoretical researches due to, mainly, the enormous technological potentiality of these materials besides being able to be manipulated, using appropriate procedures of synthesis, to present specific electronic and optic properties. Fluorenes and its derivatives is a class of polymeric materials that contain two condensed units of phenyl to a ring of five carbons in the middle, consequently, are planar monomers. These polymers have been also studied as blue light emitting devices. In this work we present some preliminary results gotten with semiempirical AM1 and PM3, as well as ab initio HF methods of quantum chemistry to analyze the influence of some substituents introduced into monomeric unit of fluorene. All used methods had shown that the introduction of a phenyl ring into fluorene monomer decrease significantly the energy GAP(H-L) and this difference still became smaller with the introduction of a ring of tetrafluorophenyl, regarding to fluorene monomer. These information are important for the understanding of the behavior of these monomers, as well as for the improvement and planning of new materials able to display properties for specific purposes.

F-P019   THE STRUCTURE ANALYSES AND CHEMISTRY PROPERTY OF METAL-ORGANIC FRAMEWORKS

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The new classes of pouros materials have been developed from ligand-bridged metal-organic compounds. Metal-organic materials (IRMOFs – isoreticular metal-organic frameworks) may have a potential impact as novel, highly effective recognition, separation, adsorption and catalytic materials due to theirs cage-like structure, the simplicity of their synthesis via self assembly and their strucutral diversity. The molecular structures of the $Zn_4O(RCOO)_6$, $R = CH_3$ and Ph, complexes, the model compounds $(CH_3COO)_5(Zn_4O)(OOC-C_6H_3X-COO)_6(Zn_4O)(CH_3COO)_5$, $X = H$, Br and NH_2, which represent an capped edge of the unit cell, and the methyl capped unit cells of IRMOF-1, -2 and -3 were calculated with AM1 and PM3, with HF/6-31G and HF/6-31G**, with B3LYP/6-31G and B3LYP/6-31G**, and with the two-layers ONIOM(HF/6-31G:PM3) methods. The diferents IRMOF´s analysed presented identical global cubic strucutrure, whereas the potential surface energy show change upon the chemistry enviroment. Comparisons with crystallographic results show that these structures were fairly well reproduced by the semiempirical methods and very well reproduced by the HF and B3LYP methods. The two-layers ONIOM (HF/6-31G:PM3) method is appropriate for structural calculations, and improvements at the ab initio or DFT level yields a methodology that can properly describes the interaction between a sorbate and the edge of the IRMOF cavities.

F-P020   RHF AND B3LYP STUDY OF LEWIS AND BRÖNSTED INTERACTION OF PYRIDINE OVER Nb_2O_5

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Lewis and Brönsted acid sites on solid surfaces are crucial for adsorptive and catalytic applications. The metal oxides surfaces consist of coordinatively unsaturated metal atoms (Mz+ cations) and oxide ions (O^{2-} anion), which are usually terminated by hydroxyl (OH-proton donor) groups. In general, these hydroxyl groups could be eliminated with high temperature treatments. The interaction between base probe molecules and preferential (Lewis and Brönsted) acid sites has different strength for the individual sites. We have studied the interaction of pyridine on oxide surface in order to characterise the Lewis and Brönsted acid sites. Ab initio RHF and B3LYP density functional methods were employed at 3-21G* basis set level and LanL2DZ ECP and basis set. Cluster models of Nb_2O_5 were built using the crystallographic data set. All geometric parameters are fully optimised. The vibrational frequencies of adsorbed pyridine were also calculated at RHF/3-21G* level.

F-P021   ROOM TEMPERATURE PHOTOLUMINESCENCE OF $BaTiO_3$: JOINT EXPERIMENTAL AND THEORETICAL STUDY.

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Strong photoluminescent emission has been measured at room temperature for BaTiO$_3$ (BT) perovskite powders. A joint experimental and theoretical study has been carried out to rationalize this phenomenon. From the experimental side, BT powder samples have been synthesized following a soft chemical processing, their crystal structure has been confirmed by X-ray data and the corresponding photoluminescence (PL) properties have been measured. Only the structurally disordered samples present PL at room temperature. From the theoretical side, first principles quantum mechanical techniques, based on density functional theory at B3LYP level, have been employed to study the electronic structure of a crystalline (BT-c) and an asymmetric (BT-a) models. Theoretical and experimental results are found to be consistent and their confrontation leads to an explanation of the PL apparition at room temperature in the structurally disordered powders.

F-P022   NUMERICAL MODEL FOR SIMULATION OF HFCVD PROCESS USED FOR DIAMOND GROWTH

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The heat transfer and fluid flow in a diamond deposition reactor will examined to identify important parameters, such as temperature, pressure and fluid flow, in the HFCVD reactor configuration. Actually the reactor configuration is performed without utilizing any detailed insight of important parameter that governs the quality and deposition rate of the films.In this work the equations of conservation of mass, momentum, and energy will be solving numerically to calculate, the temperature and fluid flow fields. Using a two dimensional model with a structured and unstructured meshes. As a result we will show a velocity fields and temperature distribution inside of reactor.

F-P023   SUPRAMOLECULAR CHEMISTRY OF NITROGEN FUNCTIONALISED PHENYLENE ETHYNYLENE MACROCYCLES

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The novel properties and potential applications of shape-persistent macrocycles, based on unsaturated hydrocarbon backbones, motivate the intense efforts that are being dedicated to prepare such macrocycles with varied structures. In this work we investigated a series of piridino-functionalised macrocycles, analogous to the well defined meta-phenylene ethynylene macrocycles (m-PEM), within 1 to 6 nitrogens per molecule. The effects on the geometry and the electronic properties of these macrocycles were studied by Density Functional Theory (DFT). Supramolecular structures in this kind of systems are stabilized by different noncovalent interactions such as hydroging bonding, hydrophobic and van der Waals. We have explored the role that hydrogen and pi-pi interactions can play in promoting self-association and stabilizing these structures. On the other hand, because of the toroidal shape of PEM´s, the internal void volume allows the formation of guest-host complexes. Therefore, guided by the bridge interactions, we investigated the potential use of functionalised PEM´s in specific molecule recognition.

F-P024   SPECTROSCOPIC AND STRUCTURAL STUDIES OF DIOXINS ORIGINATED FROM PVC COMBUSTION AND THEIR RELATIONSHIP WITH TOXICITY

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There is considerable interest in the growing utilization and environmental side effects due to incorrect disposal of recycling plastic. Consequently, high energy combustion of plastic materials have attracted both social and economical interest. In addition, there has been complaints regarding the control and treatment of residuals regarding environmental effects. In this work, we have investigated the conformations and spectroscopic properties of different dioxin molecules which were obtained from PVC combustion and are very toxic. We are particularly interested in 2,3,7,8 tetrachlorinated diobenzo-p-dioxin (TCDD), the most toxic of these molecules. In order to determine the relationship between dioxins and toxicity, we investigated the conformations of a group of dioxins with known toxicities which yields their stability and structural properties. Semi empirical AM1 and PM3 results indicates that both the number and position of chlorine substituents are important. We have used ab-initio B3LYP/6-31G(d) calculations to investigate the interaction with the binding site of dioxin receptor s by analyzing the structure and energy of the TCDD-amino acid residue complex. Spectroscopic properties were also calculated and compared with experimental results from our laboratory.

F-P025   THEORETICAL AND EXPERIMENTAL STUDY OF THE PHOTOLUMINESCENCE IN DISORDERED $SrWO_4$ THIN FILMS

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The nature of visible photoluminescence at room temperature of $SrWO_4$ (SWO) thin films in their crystalline and disordered forms is studied in the light of experimental results and theoretical calculations. The SWO thin films have been synthesized following a soft chemical processing. First principles quantum mechanical techniques, have been employed to study the electronic structure of two models, symmetric one and an asymmetric one standing for the crystalline and disordered thin films. Experimental results obtained by X-ray diffraction data and photoluminescence measurements reveal that the photoluminescence increases with the degree of disorder in SWO thin film. The UV-vis optical spectra and the calculations indicate that the structural disorder of SWO creates localized electronic levels in the band gap. From theoretical data, it has been noticed that a negative charge transfer process takes place from threefold cluster $[WO_3]$ to regular tetrahedra cluster $[WO_4]$. The charge polarization induced by the symmetry break in the disordered structures and the existence of locallized levels auxiliates the creation of trapped holes and electrons, giving the origin of the room temperature photoluminescence phenomenon.

F-P026 STRUCTURAL AND ELECTRONIC PROPERTIES ON PBTIO$_3$: DENSITY FUNCTIONAL THEORY APPLIED TO PERIODIC MODELS

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Calculations based on density functional theory at the B3LYP hybrid functional level applied to periodic model have been performed to characterize the structural and electronic properties of PbTiO$_3$. Two different slab terminations (PbO and TiO$_2$) have been done to obtain and discuss the results of band structure, density of states, charge distribution on bulk and surface relaxation. It is observed that the relaxed processes are most prominent for the Ti and Pb surface atoms. The electron density maps confirm the partial covalent character of the Ti-O bonds. The calculated optical band gap and other results are in agreement with experimental data.

F-P027 MAGNETIC PROPERTIES OF MnAs INTERMETALLIC COMPOUNDS AT ZERO AND MAGNETIC TRANSITION TEMPERATURES.

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The MnAs intermetallic compound crystallizes in the NiAs (B81) structure, a ferromagnetic hexagonal phase and in the MnP (B31)structure, a non magnetic orthorhombic phase. In this work we investigate theoretically the magnetic behavior of this compound in the ferromagnetic phase at zero and magnetic transition temperatures. The study was done using Wien 97 code, all electron full potential linearized augmented plane wave method (FPLAPW) with spin polarized energy band calculations based on density functional theory (DFT) with general gradient approximation (GGA). For this material the calculated spin magnetic moment at Mn site is 3.86 µB and at the As site is 0.21 µB with a total spin magnetic moment of 3.65µB which is in a very good agreement with the experimental results. We also present in this work the total density of states, band energy dispersion curves, total energy per atom as a function of the system volume, as well as the magnetic moment as a function of the systems lattice parameter for the magnetic phase. We also present the total energy per atom for non-magnetic phases. We observed that MnAs compound in the ferromagnetic phase presents a half- metallic behavior.

F-P028   COMPUTER SIMULATION OF THE CRYSTAL STRUCTURE OF ? -ALANINE.

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The computer simulation of the crystal structure of alfa-alanine was undertaken as part of a program of research on the structures of materials of biological importance. Many experimental studies, by X-ray diffraction, of the total, static electron density in a crystal is a field of increasing interest, and many important properties can be derived including intermolecular distances, atomic and group charges, dipole and quadrupole moments, electrostatic potentials, electric field gradients, and intermolecular electrostatic energies within the crystal. Experimentally, the electron density distributions, measured by X-ray diffraction, are interpreted in terms of three types of functions: (i) spherical functions, describing the distributions of inner shell and valence electrons distribution, (ii) deformation functions, representing the aspherical distribution of the valence electrons, and (iii) anisotropic displacement parameters (ADPs), describing effects such as thermal motion, molecular librations, and other types of atomic displacements. A crucial aspect of this interpretation involves the ability to separate the ADPs (iii) from the static parameters (i) and (ii). Alanine crystallizes as a zwitterion, $NH_3^+CHCH_3COO^-$, in an orthorhombic cell, space group P2l2l2l. This work reports a comparison between calculated, by ab initio periodic method, and experimental features of the electron density, and nuclear densities as measured by X-ray and neutron diffraction, respectively.

F-P029   STRUCTURAL AND ELETRONIC PROPERTIES OF $BaZrO_3$

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In the last years, the interest for the $BaZrO_3$ material is continuously increasing. The list of the potential applications for $BaZrO_3$ is an open one and, due to this, investigations of this compound is important. Several areas in wich this material is useful are: aero-space and related industries, high temperature superconductors (HTS) and solid oxide fuel cells and sensors. Theoretical-computational studies, based on ab initio calculatons can yeld important information regarding the electronic and structural properties of solids. This technique provides a framework for the interpretation of experimental data. At this sense, structural and eletronic properties of the bulk and relaxed surfaces (ZrO_2 and BaO (100) termination) of cubic phase (space group Pm3m) of $BaZrO_3$ are investigated by means of periodic quantum-mechanical calculations based on density functional theory. It is observed that the diffference in surface energies is small and relaxations effects are most prominent for Ti and Zr surface atoms. The eletronic structure shows a splitting of the lowest conduction bands for the ZrO_2 terminated surface and of the highest valence bands for the BaO terminated slab.

F-P030   AN INVESTIGATION OF THE ORDERING TRANSITION IN EQUIATOMIC FeRh COMPOUND.

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Among the various systems that are candidates for application as magnetostrictive transducers is the intermetallic compound FeRh. The iron-rhodium compounds are known to exhibit a large induced volume magnetostriction, at and above room temperature, and are na example of the anti-Invar behavior. The equiatomic FeRh alloy is an interesting system in which both Invar and anti-Invar effects qre present in different range of temperatures, being that the Invar-like behavior is observed at and below the ordering temperature and has been mainly attributed to transverse fluctuation of the local magnetic moments. Otherwise the anti-Invar behavior observed at the ferromagnetic-antiferromagnetic transition is attributed to the colapse of the local rhodium moment as a consequence of the longitudinal spin fluctuation at low temperatures. Recently the experimental results have shown that the ferromagnetic-antiferromagnetic transition showed by FeRh alloys is replaced by a new transition between two different ferromagnetic phases at low temperatures. In this work we performed electronic structure calculations with the molecular cluster discrete variational method to study the magnetic transitions in the FeRh alloy.

F-P031   SUPERCONDUCTIVITY OF M-B_2 DIBORIDES, M = Al, Ti, V, Cr, Zr, Nb, Mo AND Ta

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The crystal structure of MB_2 (s.g. $D3\_\{3d\}$ or P6/mmm) is a graphite-structured hexagonal nets of B atoms (honeycomb lattice), separated by hcp layers of M atoms. Several metallic borides possess the AlB_2-type structure. Since the first studies of the bonding properties of metals, the isostructural borides have been adopted to attempt to correlate the internuclear separations with the bond radius assigned to the metal consistent with the valence modified by charge transfer. The single-bond radius of boron was expected to vary inversely with the valence of boron, and is very sensitive to the amount of p- and d-character assigned to the bond orbitals. In this work first-principles molecular clusters calculations were performed to study the superconductivity of M-B_2 compounds. Pressure effects on the density of states at the Fermi level were investigated for both magnesium and boron atoms in this compound. In the M-B_2 diborides, M = Al, Ti, V, Cr, Zr, Nb, Mo and Ta, the largest contributions to the DOS at the Fermi level is observed for Cr, Mo and Nb. The TiB_2 has the highest chemical stability in the series. The investigation of the effect on the DOS at the Fermi level with the introduction of a monolayer of solute atoms in the Mg sites shows the formation of a pseudogap near the Fermi level in these compounds.

F-P032   A STUDY OF THE MAGNETIC PROPERTIES OF THE OsFe$_3$N NITRIDE.

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The iron nitrides have been intensively studied in the last past years in view of their potential applications for high density magnetic recording. Fe$_4$N crystallizes in a perovskite-like structure, where the Fe atoms occupy two sublattices, namely, corner sites (FeI) and face centered sites (FeII), with the N atoms located at body centered sites. Among the several candidates which have been investigated for structural substitutions for iron, the 5d elements have provided a subject for an intensive research, as an attempt to enhance the performance of these compounds for practical purposes. In this context, the Os substitution have been investigated with various experimental techniques. From these was verified that the lattice parameter is not changed with the substitution for the FeI sites. Results of Mössbauer spectroscopy measurements have indicated that osmium preferentially substitutes for Fe at the corner (FeI) sites. In this work the full potential-linearized augmented plane wave (FP-LAPW) method based on density functional theory is employed to investigate the electronic structure of the OsFe$_3$N nitride. From the calculations we obtained the local magnetic moments as well as the hyperfine magnetic fields for the metal sublattices and for the N atoms.

F-P033   VORTEX DYNAMICS IN THIN TYPE-II SUPERCONDUCTING STRIPES WITH PERIODIC PINNING

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Using Molecular Dynamics, we study the collective motion of vortex lattices in thin type-II superconducting stripes. The two dimensional stripe of thickness less than the penetration depth, has an edge barrier in the longitudinal direction, and is infinite in the transverse direction. The numerical simulations are performed using the Langevin equation, and we include the vortex-vortex interaction, the vortex interaction with the surface current, vortex images and a periodic pinning arrangement. The vortices trajectories and the differential resistivity are calculated and compared with the case of random pinning.

F-P034   USE OF THERMODYNAMIC SIMULATION AT PREPARATION OF PURE OPTICAL GERMANATE AND TELLURITE GLASSES

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GeO_2 - and TeO_2-based optical glasses are perspective materials for the making of broad band fiber optics amplifiers for S and L bands of optical communication. Technology of single-mode fibers impose very strict requirements to the purity and optical homogeneity of these glasses. The glasses must be free of impurities of light elements, in the first turn from molecular H_2O, CO_2 and OH^- groups. These impurities have also negative influence on emission characteristics of the glasses doped by rare earth elements (REE). Presence of H_2O, OH- and CO_2 impurities can decrease significantly lifetimes of exited states of REE at luminescence. Thus, problem of the glass purification from these impurities is of a primary importance. Thermodynamic computer simulation of high temperature chemical equilibrium in GeO_2 and TeO_2 based glass melts was used for finding of optimal temperature conditions of glass preparation. The simulation is based on a fundamental principle of enthropy maximum. Experimental data on pure GeO_2- and TeO_2-based glass preparation are given. Possible chemical forms of transition metal impurities are also discussed on the base of results of the thermodynamic simulation. Thus, thermodynamic simulation seems to be a useful way for predicting of glass melting conditions as well as for evaluation of the composition of the initial glass components mixtures at preparation of pure optical homogeneous glasses, especially in the goals of fiber optics.

F-P035   MODELING COMPOSITE FIBROUS-MATRIX SYSTEMS BY COMPUTER SIMULATIONS

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Composite materials can be defined as a macroscopic combination of different substances, which interfacial contact. With this kind of composition, composite materials have non-continuous phase: one is responsible for the mechanical properties and the other responsible for the integrity of them. The matrix maintains also the position – or orientation - of the reinforcement substance (fibers, particles etc). Nowadays, this class of materials has a large range of applications, and their use is widespread in many types of industrial projects. So, it is important to understand their mechanical properties, as their behavior under extreme stress and consequent fracture. The goal of this work is to simulate the failure process of fiber reinforced composites. In our model, we suppose that the fibers are fixed in a parallel direction. Different from others previous works, where a broken fiber does not support any load, we assume explicitly the existence of the matrix, and some types of fracture processes can be studied. In this model, we also study the effects of temperature and loading velocity on the fracture. The complete failure of the material occurs by fusion of many cracks, when a surface is formed. The probability of rupture of a fiber depends on the existence of unbroken neighboring fibers (which share a local load) and is given by a Weibull distribution.

F-P036   A NEW CLASS OF PUSH-PULL MOLECULES FOR MOLECULAR ELECTRONICS

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A new class of push-pull molecules is constitutive by betaine. It one designates not only the $[(CH_3)_3N^+ CH_2COO^-]$ molecule, but also several quaternary ammonium salts analogous in structure. Pyridinium betaines are good candidates for the design of photoactive molecular assemblies and the preparation of LB films with intense NLO response. Small pyridinium betaines have large molecular hyperpolarizabilities relative to their molecular sizes. Since experimental data are not available for the geometries of the molecules investigated, systematic geometry optimizations were required. In this work we report an electron transfer of known betaines class of molecules. Using semiempirical including CI and density functional theory methodology we founded that for conjugated chain as intermediary of donor/acceptor groups. We have carried out INDO/S-CI calculations using on the average 220 configurations (singlet/triplet) with the geometries obtained from ground state calculations. Our results show an net charge transfer as the photoinduced electronic flow that it does not follow the standard direction; rather, it happens in a reversed manner, from the acceptor to the donor side of the molecule. This behavior is associated to a corresponding inversion of the spatial localization of the frontier molecular orbitals.

F-P037   AN ALTERNATIVE WAY OF MODELLING DOPED MATERIALS

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The addition of dopant in a ceramic host lattice yields a great interest in nowadays chemistry because of the great range of peculiar properties they allow to tune in fields as diverse as electrical, optical, structural, and mechanical properties.

Theoretical studies of those doping-enhanced properties are of first interest for understanding their intrinsic origin. However, it is very difficult to model a doped material. The usual way is to create a huge supercell by multiplying the original unit cell, and then to substitute one of the cell-constituting atoms by the doping element. This multiplication of the unit cell is mandatory in order to introduce the doping element in reasonable proportions. Even this way, its effect on the electronic structure acts as a mask, it is overestimated. In this work, we are proposing an alternative method, based on experimental structural characterization from X-ray diffraction data. The periodic models we use in our DFT calculations at B3LYP level are taken from a very accurate Rietveld refinement of a pure and a doped $BaTiO_3$ synthesized by the polymeric precursors method. This model gives access to the dopant general effect on the electronic behavior. In fact, the influence of the doping element itself on the electronic configuration is barely local; therefore, it is not included in the simulation. The results are confronted to experimental measures like optical gap, photoluminescence, tetragonality of the unit cell and the accordance.

F-P038   SIMULATION OF SMALL MOLECULES THROUGH CARBON NANOTUBES

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Understanding the diffusion of gas molecules in nanomaterials is important for technological applications. Many research groups have studied the carbon nanotubes and the diffusion of hydrogen, nitrogen and hydrocarbons. The nanometer scale of carbon nanotubes and cylindrical shape induces their potential technological and industrial applications, e.g., hydrogen storage. Carbon nanotubes are constructed of chemically opened nanotubes that are arranged in a close-packed structure. Therefore, we have performed computational molecular dynamics and molecular mechanics simulation of light hydrocarbons, in order to study the movement and adsorption of ethane, propane and buthane gas molecules through carbon nanotubes at room temperature. We have used CHARMM, UFF, OPLS AMBER and MM3 molecular mechanics force fields in order to model the gas molecule adsorption

F-P039   A PERIODIC DFT STUDY OF THE LI MOBILITY IN THE TIO_2-ANATASE STRUCTURE

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Li ion secondary battery is widely applied to electronic devices used in our everyday life, because of its high energy density and rechargeability. Due to the fact TiO_2 is a lightweight, inexpensive material, and having favourable sites for Li insertion, it can be considered as a potential material for lithium ion secondary batteries. In this study different concentrations of Li-doped TiO_2-Anatase crystal structure were investigated on their respective ion mobility. The calculations were performed using density-functional theory employing ultra-soft pseudo-potentials, a plane wave basis set, and the PW91 density functional. The geometries of the crystals used are optimized and the results for different Li-concentrations are compared where possible with experimental data. Consequently, activation barriers for the ion mobility between the different interstitial spaces available (tetrahedral and octahedral) are calculated, and approximated diffusion rate are presented.

F-P040 AB INITIO THEORETICAL APPROACH AND PREDICTION OF NEW METALLIC CATALYSTS FOR DESULPHURIZATION OF THE DIBENZOTHIOPHENES DERIVATIVE COMPOUNDS

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Recently, the interest in the deep hydrodesulfurization (HDS) of gas oil has been renewed due to the stricter regulations concerning the sulfur content in diesel oil. In order to protect the global environment, many countries have lowered the limit of the sulfur content of gas oil to 0.05%. Trends show that these countries will have lowered the limit to 0.005% (50 ppm) in the near future. To meet this assignment, the development of a suitable catalyst for the deep HDS of gas oil is a very important subject. When gas oil was desulfurized with a conventional HDS catalyst, the most refractory sulfur compounds were found to be dibenzothiophenes derivatives. In order to develop a fundamental understanding of the HDS method, as well and adsorption mechanism of thiophenic compounds 4,methyl-dibenzothiophene (4-MDBT) and 4,6-dimethyl-dibenzothiophene (4,6-DMDBT) over transition metals clusters, a molecular simulation of these thiophenic compounds over metallic matrix has been performed using Ab initio theoretical approach. A fundamental understanding of the HDS active sites and the mechanism of such catalysts is essential for developing efficient catalysts and processes. Strong interactions between thiophenic compounds and metallic catalysts were observed, especially in the sulfuric sites with some metals of 2nd transitions series.