MMN'2018

01-04 October 2018

2ND INTERNATIONAL WORKSHOP ON MAGNETIC MATERIALS & NANOMATERIALS MMN'2018

BOOK OF ABSTRACTS

BOUMERDES-ALGERIA
01-04 OCTOBER 2018

Second International Workshop on Magnetic Materials and Nanomaterials

MMN'2018

Boumerdes, Algeria

01-04 October, 2018

Workshop Organizer:

Physics department, Faculty of Sciences,

M'Hamed Bougara University of Boumerdes, UMBB

TABLE OF CONTENTS

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Preface

The second international workshop on Magnetism and Magnetic Nanomaterials, MMN'2018, will be held from 01 to 04 October 2018 at Physics department, Faculty of sciences, M'hamed Bouguerra University of Boumerdes (UMBB). This event MMN'2018 is organized by the group of magnetic materials belonging to URMPE, UMBB. The main objective of this workshop is ensure an exchange of the latest research works performed in the field of magnetic materials and nanomaterials. This exchange will initiate future collaborations that will be beneficial for our students and researchers in Algeria.

For this second edition MMN'2018, more than 120 participants coming from 11 european countries and 26 Algerian cities will be present. In this book, we have collected the extended abstracts (Plenary, oral and poster) with their references. The arrangement of time presentation of 30 minutes for plenary talks and 15 minutes for the oral presentations will permit an exchange of the latest results in the field of magnetic materials and nanomaterials.

The selected papers will be published, after a peer reviewed according to standard international procedures, in the journals: hyperfine interactions and SPIN. I would like to adress a special thanks to Prof. Guido Langouche and Prof. Yeow-Hwa for consacring special issues to MMN'2018. This will undoubtedly give credibility to our workshop and contribute to raising its scientific level.

The organization of this workshop was not possible without the valuable contribution of the sponsors. I would like to adress a hugh thanks to the sponsors (CRNA, CRNB, SONELGAZ, ATRST) for their fiancial support.

Finally, I would like to thank all invited speakers, contributors, session chairs and the members of scientific committee for their effort in making MMN'2018 workshop a successful meeting.

Welcome in Boumerdes, Algeria, October 2018

Dr. A. Guittoum,
Nuclear Research Centre of Algiers, Algeria
Chairman (Algeria)

SCIENTIFIC PROGRAM

October 01, 2018 (afternoon)			
14h00-19h00	**Registration, Reception, Official opening ceremony: 17 h**		
October 02, 2018			
9h00- 11h15	**Topic 04: Theory and modeling in magnetism Chairman: Prof. R. Schäfer**		
9h00- 9h30	PL01-T04	S. Lounis	Single magnetic skyrmions from first-principles: from pinning effects to electrical and x-ray reading
9h30- 10h00	PL02-T04	S.Bonetti	Terahertz probing and manipulation of magnetism
10h00-10h30	PL03-T04	S. Sanvito	End-to-end materials discovery with electronic structure theory and machine learning
10h30-10h45	O01-T04	H. M. A. Mazouz	First-principles prediction of lattice dynamics and thermal properties of rocksalt half-metallic ferromagnets: case of NaO and KO
10h45-11h00	O02-T04	D. Brinis	Dynamics of magnetization in the assemblies of ferromagnetic nanoparticles : Effect of interactions
11h00-11h15	O03-T04	T. Rezkallah	Electronic and magnetic properties of Mn doped ZnO using the FP-LAPW approximation
11h15-11h30	**Coffee Break**		
11h30- 13h00	**Topic 02 : Mössbauer spectroscopy in magnetic materials Chairman: Prof. G. Langouche**		
11h30- 12h00	PL04-T02	J. M. Greneche	Fe-based nanomaterials investigated by ^{57}Fe Mössbauer spectrometry
12h00- 12h30	PL05-T02	A.Kamnev	Ferritins as natural magnetic nanomaterials: Mössbauer spectroscopic monitoring of iron transformations in bacterial cells
12h30-12h45	O04-T02	N. Boukherroub	Microstructure, hyperfine and magnetic properties of nanostructured $(Ni_{75}Fe_{25})_{100-x}Si_x$ alloy elaborated by mechanical alloying
12h45-13h00	O05-T02	O. Ould Fella	Microstructural and Magnetic Properties of Zinc ferrite and Annealed zinc ferrite Nanoparticles by Means of X-Ray Diffraction and Mössbauer Spectroscopy
13h00-14h30	**Lunch**		
14h30-16h45	**Topic 01: Elaboration of magnetic thin films and nanomaterials Chairman: Prof. S. Lounis**		
14h30-15h00	PL06-T01	J. Vejpravova	Internal spin architectures in nanoparticles
15h00-15h30	PL07-T01	P. Gorria	End-to-end materials discovery with electronic structure theory and machine learning Exploring magneto-volume anomalies and magneto-caloric effect in R_2Fe_{17} intermetallic alloys

15h30-16h00	PL08-T01	I. Chicinas	Soft magnetic nanocrystalline powders and nanocrystalline/composite compacts obtained by mechanosynthesis and spark plasma sintering
16h00-16h15	O06-T01	A. Kaibi	Microstructure, hyperfine and magnetic properties of nanostructured $(Ni_{75}Fe_{25})_{100-x}Si_x$ alloy elaborated by mechanical alloying
16h15-16h30	O07-T01	M. Mebarki	Effect of the elaboration techniques and the porosity of the substrate on the structural and ma properties of Fe films deposited on Al
16h30-16h45	O08-T01	D. Lakhdari	Elaboration and characterization of NiFe thin films
16h45-17h00	Coffee break		
17h00-19h00	Topic 04: Theory and modeling in magnetism Chairman: Prof. S. Sanvito		
17h00-17h15	O09-T04	Y. Bensaidane	Giant magneto-resistance in the CoCuCo magnetic junctions
17h15-17h30	O10-T04	I. Djabri	Structural, electronic, optical, and magnetic properties of Co-doped Cu_2O
17h30-17h45	O11-T04	D. Aissat	The effect of geometric anisotropy on transport properties in spintronic junction based on MnPt Connected to a noble metal lead
17h45-18h00	O12-T04	Z. Abdelli	Ab initio electronic structure calculations of half-metallic ferromagnetism in diluted magnetic semicond based GeTe
18h00-18h15	O13-T04	Y. Boulbenza	Electronic and magnetic study of new diluted semiconductors
18h15-18h30	O14-T04	A. Labdelli	Investigation of the magnetic and optoelectronic properties of the perovskite $GdRuO_3$ using DFT+U with spin-orbit coupling
18h30-18h45	O15-T04	M. A. Ghebouli	Spin-Polarized structural, electronic and magnetic properties of diluted magnetic semiconductors $Ca_{0.75}TM_{0.25}O$ (TM = Fe, Co and Ni) in the rock salt (B1) phase
18h45-19h00	O16-T04	H. B. Benziane	Magnetic exchange interaction of Mn_2SnTe_4
October 03, 2018			
9h00- 11h15	Topic 03: Properties of magnetic thin films and nanomaterials Chairman: J. M. Greneche		
9h00- 9h30	PL09-T03	R. Schäfer	Micromagnetism, Magnetic Microstructure and their Magneto-Optical Analysis
9h30-10h00	PL10-T03	W. A. A. Macedo	Magnetic anisotropy and coupling in Fe-based layered nanostructures
10h00-10h30	PL11-T03	M. Kalbac	Magneto-Raman spectroscopy-a great tool for studying the coupling of magnetic excitations to phonons

10h30-10h45	O17-T03	N. Mansouri	Physicochemical and magnetic properties of $Fe_{50}Co_{50}$ nanowires electroplated in alumina membranes
10h45-11h00	O18-T03	T. Kacel	Influence of the thickness on structural, electrical and magnetic properties of Ni films electrodeposited onto n-Si (100) substrates
11h00-11h15	O19-T03	M. Hocine	Effect of the milling time on structural and magnetic properties of $(Fe_{0.7}Co_{0.3})_{95}Si_5$ alloy obtained by mechanical alloying
11h15-11h30	Coffee break		
11h30-13h15	Topic 04: Theory and modeling in magnetism Chairman: J. Vejpravova		
11h30-12h00	PL12-T04	N. Baadji	charge, spin and heat current in magnetic tunnel junction
12h00-12h30	PL13-T04	L. V. Dobysheva	First-Principles Calculations for Alloyed Cementite (Fe–Ni-Cr)3C
12h30-12h45	O20-T04	R. Tigrine	Localized energies and state density at the alloy surface
12h45-13h00	O21-T04	M. A. Lahmer	Long-range antiferromagnetsim in Fe-doped $ZnAl_2O_4$: a first-principles study
13h00-13h15	O22-T04	O. Hamidane	First-Principle Predictions of Electronic Properties and Half-Metallic Ferromagnetism in Vanadium-Doped Rock-Salt SrO
13h15-14h30	Lunch		
14h30-17h15	Topic 01: Elaboration of magnetic thin films and nanomaterials Chairman: A. A. Kamnev		
14h30-15h00	PL14-T01	V. Kuncser	Magnetism and magneto-optical effects in rare-earth based amorphous-like compounds
15h00-15h30	PL15-T01	S. Farhat	Graphene synthesis via plasma enhanced CVD and magnetic induction
15h30-16h00	PL16-T01	A. Espinosa	Magnetic nanoparticles-mediated thermal therapies: quantitative comparison of heat generation, therapeutic effiency and limitations
16h00-16h15	O23-T01	Y. Gaci	Effect of Fe content on the structural and magnetic properties of ternary $(Ni_{60}Co_{40})_{100-x}Fe_x$ nanoparticles synthesized by hydrothermal route
16h15-16h30	O24-T01	M.Salhi	Elaboration of Nickel films by PVD : method and procedure
16h30-16h45	O25-T01	D. Grine	Deposition of TiO_2/Fe_2O_3 composite thin films by vacuum thermal evaporation
16h45-17h00	O26-T01	A. Hayoune	Synthesis and characterization of magnetic iron oxide/clay composite and its application for methylen removal
17h00-17h15	O27-T01	M. Mhadhbi	Structural and magnetic properties of nanostructured $Fe_{60}Al_{40}$ powders prepared by mechanical alloying
17h15-17h30	Coffee break		
17h30-19h30	Poster session		

October 04, 2018			
9h00- 11h00	**Topic 03: Properties of magnetic thin films and nanomaterials Chairman: W. A. A. Macedo**		
9h00-9h30	PL17-T03	S. M. Chérif	Dzyaloshinskii-Moriya interaction in ultrathin magnetic stacks: a route toward future spintronic
9h30-10h00	PL18-T03	A. Cheikhrouhou	Magnetic and magnetocaloric properties of RM_2 laves phases compounds (R = Er, Tb, Ho and M = Fe, Co, Mn)
10h00-10h15	O28-T03	S. Bahamida	Structural and magnetic properties of $Fe_{64}Pd_{36}$ films deposited onto glass and Si (100) substrates
10h15-10h30	O29-T03	K. Cheraitia	Analysis of impurities of Nd-Fe-B Magnet by nuclear method and recovery by precipitation chemical of N Pr rare earths
10h30-10h45	O30-T03	N. Djellal	Effect of lanthanum substitution on cobalt ferrite structural and magnetic properties
10h45-11h00	O31-T03	H. Oubouchou	Elastic modeling of spin-cossover nanocomposites: towards multi-sptep spin transitions
11h00 – 11h15	**Coffee break**		
11h15-13h00	**Topic 05: Magnetism for engineering and environment Chairman: Prof. V. Kuncser**		
11h15-11h45	PL19-T05	E. Hristoforou	Selective magnetic separation for sewage and desalination
11h45-12h15	PL20-T05	N. Fenineche	Microstructure and Magnetic Properties of FeNi and FeSi Alloys using additive manufacturing Process
12h15-12h30	O32-T05	D. Ouadjaout	Numerical analysis of induction heating in a crystal pulling-CZ furnace
12h30-12h45	O33-T05	S.Aguib	Modeling of magnetic force and identification the magneto-mechanical properties of elastomer
12h45-13h00	O34-T05	W. Rezig	Preparation, Characterization and valorization of Hydroxide Ferric (III) Modified Aluminosilicate Kieselgu Material
13h00-13h30	**Closing ceremony**		
13h30-14h30	**Lunch**		
14h30-20h00	**Excursion around Algiers city**		

PLENARY LECTURES
INVITED SPEAKERS

PL01-T04
SINGLE MAGNETIC SKYRMIONS FROM FIRST-PRINCIPLES: FROM PINNING EFFECTS TO ELECTRICAL AND X-RAY READING

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ABSTRACT

Magnetism is a fascinating correlation phenomenon with ramifications over several orders of magnitude in length and timescale. It generates thrilling questions across multiple fields rooting in condensed matter physics with paramount implications in information technology. The quest for new paradigms to increase computing speed and storage capacity at reduced energy footprint hinges on the fundamental understanding of microscopic mechanisms underlying the stability, detection and manipulation of nanoscale magnetic elements in a material specific context. This requires novel concepts, the development of cutting edge methodologies and surmounting formidable computational challenges. In this talk, I present a few highlights from our current researchbased on first-principles and related to magnetic skyrmions, which are particles-like spin textures generating a lot of interest because of their rich physics and technological potential for future information and communication devices. Such magnetic entities have a topological nature providing a link between topology and spintronics.Their nucleation, motion and velocity are, however, heavily affected by materials inhomogeneities ubiquitous to any device. Thus, a detailed knowledge of defects-skyrmion interactions is desirable but unknown, which limits the realization of such topological magnetic entities as possible bits of information.I will address this issue and demonstrate that skyrmions can either be expelled or pinned depending on the chemical nature of impurities. [1] we quantify the defects-skyrmion interactions and demonstrate the universality of its pattern as function of the filling of the impurities electronic states.Then I will discuss ab-initio-inspired protocols to detect magnetic skyrmions either electrically – via the tunnelling spin-mixing resistance (TXMR) [2, 3] or with soft X-ray spectroscopy–by measuring the counterintuitive topological orbital moment carried by skyrmions [4, 5].

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PL02-T04

TERAHERTZ PROBING AND MANIPULATION OF MAGNETISM

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ABSTRACT

The interaction between magnetism and light is receiving considerable interest in recent years, after the ground-breaking experiments that showed that ultrashort (~100 fs) infrared light pulses can be used to demagnetize or even switch the magnetization of thinnanometerfilm ferromagnets [1]. However, to date no clear and commonly accepted understanding of the fundamental physical processes governing the ultrafast magnetization has been reached, partly because accurate modelling of the infrared fs laser-induced highly non-equilibrium state remains a key obstacle. It has recently been shown that not only infrared, but also terahertz light pulses can be used to observe ultrafast demagnetization in thin film ferromagnets [2]. In addition, terahertz radiation can be used as a probe of the fundamentals of spin transport [3]. In this talk, I will go through some basic and more advanced concepts in the exciting emerging field of terahertz (THz) magnetism, where electromagnetic radiation in the 0.1-10 THz range, the so-called THz gap, is used to probe or to control spin dynamics in thin ferromagnetic metallic films at these time scales. I will also show some recent implementation of metamaterials aimed at selectively enhancing the terahertz magnetic field in the near-field [4], with the goal of realizing the first table-top precessional or “ballistic” magnetization switching, the fastest possible spin reversal mechanism.

References

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PL03-T04

END-TO-END MATERIALS DISCOVERY WITH ELECTRONIC STRUCTURE THEORY AND MACHINE LEARNING

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ABSTRACT

The development of novel materials is a strong enabler for any technology, and often technology and materials innovation cannot be separated. Unfortunately the process of finding new materials, optimal for a given application, is lengthy, often unpredictable and has a low throughput. Here I will describe a systematic pathway to the discovery of novel materials, which demonstrates an unprecedented throughput and discovery speed. The method can be applied to any materials class and any potential application. I will use the example of magnetism to introduce the main features of the method, and I will demonstrate the discovery of several new high-performance magnets. Furthermore I will highlight how such high-throughout schemes can be combined with machine-learning methods for data-mining to extract novel materials designing rules and for identifying new prototypes for further investigation. Based on an extensive electronic structures library of Heusler alloys containing 236, 115 prototypical compounds, we have filtered those alloys displaying magnetic order and established whether they can be fabricated at thermodynamical equilibrium. Specically, we have carried out a full stability analysis for in-termetallic Heuslers made only of transition metals. Among the possible 36, 540 prototypes, 248 are found thermodynamically stable but only 20 are magnetic. The magnetic ordering temperature, T_C, has then been estimated by a regression calibrated on the experimental T_C of about 60 known compounds. As a final validation we have attempted the synthesis of a few of the predicted compounds and produced two new magnets. One, Co_2MnTi, displays a remarkably high T_C in perfect agreement with the predictions, while the other, Mn_2PtPd, is a complex antiferromagnet. Our work paves the way for large-scale design of novel magnetic materials at unprecedented speed.

References

Stefano Sanvito, Corey Oses, Junkai Xue, Anurag, Tiwari, Mario Zic, Thomas Archer, Pelin Tozman, Munuswamy Venkatesan, J. Michael D. Coey and Stefano Curtarolo, Accelerated discovery of new magnets in the Heusler al loy family , Science Advances 3, e1602241 (2017).

PL04-T02

FE-BASED NANOMATERIALS INVESTIGATED BY ^{57}FE MÖSSBAUER SPECTROMETRY

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ABSTRACT

For the last decades, great attention has been widely devoted to the development of nanosciences and nanotechnologies because of both fundamental aspects and potential applications. The structural, chemical and physical properties of the nanomaterials which include nanoparticles, multilayers, nanoarchitectures must be carefully investigated to establish size dependent structure-physical properties correlations. Such a step remains highly delicate and requires multi-scale characterization techniques including diffractions, electron microscopies and local probe spectroscopies while magnetic measurements in different conditions have to be performed in the case of magnetic nanostructures. In addition, computer modelling is now suitable to bring very useful and complementary information. Consequently, the strategy consists first in a fine and deep characterization of these magnetic nanomaterials using complementary techniques, and then in the modelling of structural and magnetic properties to better understandintrinsec phenomena such as surface and interface effects, exchange bias and the role of dipolar interactions. After a short description of 1D, 2D and 3D nanostructures, and some general features of Mössbauer spectroscopy, we illustrate the presentation with several selected examples based on nanocrystalline alloys, nanostructured powders nanoparticles and hollow magnetic nanostructures.

PL05-T02

FERRITINS AS NATURAL MAGNETIC NANOMATERIALS: MÖSSBAUER SPECTROSCOPIC MONITORING OF IRON TRANSFORMATIONS IN BACTERIAL CELLS

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ABSTRACT

Ferritins are members of a superfamily of specific proteins, with nano-sized iron(III)-bearing cavities (mineral “iron cores”) within proteinaceous shells, ubiquitous in virtually all organisms, presenting a variety of nanobiotechnological applications. They represent natural water-soluble ‘reservoirs’ of iron with not yet completely known functions, properties and mechanisms of functioning of their ferroxidase centres. Iron is accumulated in the core and stored in the form of Fe^{III} oxyhydroxides of different crystallinity and variable composition (in bacteria, as phosphate-rich and less crystalline Fe^{III} oxyhydroxides). In this keynote lecture, Mössbauer spectroscopic data will be presented and discussed featuring the metabolic redox transformations of iron, sequestered from the culture medium by live bacterial cells (using the example of the ubiquitous widely studied plant-growth-promoting rhizobacterium *Azospirillum brasilense*), for up to 10 days. Significant reduction of $^{57}Fe^{III}$ (in the form of its NTA complex in the culture medium) to $^{57}Fe^{II}$, detected in rapidly frozen cells separated from the culture medium as two high-spin forms, upon iron assimilation by cells was observed throughout the storage period, with the simultaneous presence of a $^{57}Fe^{III}$-containing ferritin-like species as one of the components in the spectra with broadened lines. This assignment was complemented by room-temperature high-velocity-resolution and low-temperature (including in-field) Mössbauer measurements on lyophilised biomass of A. brasilense. At T≤5K, a broadened magnetically split sextet was observed in Mössbauer spectra which corresponded by its parameters to bacterial ferritins studied in other bacteria. In addition, besides a relatively small residual ferrous component, there remained a noticeable superparamagnetic quadrupole-split component of iron(III) which might represent ferric complexes other than the ferritin core and/or superparamagnetic ferritin species with small core sizes (with a lower blocking temperature) [4] in the intracellular iron pool.

Acknowledgements. The author is grateful to the MMN-2018 Organisers for their invitation and support of his participation in the Workshop. This work was supported in part by the Russian Foundation for Basic Research (Project 17-08-01696-a).

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PL06-T01

INTERNAL SPIN ARCHITECTURES IN NANOPARTICLES

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ABSTRACT

Magnetic nanoparticles are the fixed stars in the sky of modern magnetism due to their multifaceted application potential. The control over their functional properties can be generally maintained on three levels: the atomic level (elemental composition, defects), the single-particle level (single-domain vs. multi-domain, core-shell and beyond), and the mesoscopic level (inter-particle interactions and size distribution) [1, 2]. So far the main challenge is to master the particle architecture at the single particle level as the relationship between the degree of the particle crystallinity, spin order and magnetic response is essential; consequently the fractions of different structural and magnetic order within a single-particle are in intimate contact through an internal interface, which is a source of additional contribution to the total single-particle magnetic anisotropy. In this vein, synergy of various structural and magnetic probes for addressing the phenomena will be demonstrated on typical examples of single-domain nanoparticles with different internal architectures (highly-crystalline, natural core-shell, and artificial core-shell) and put in broader context by comparing to similar effects in other classes of nanoparticles. Finally, the importance of the internal interfaces will be discussed in the frame of potential applications like magnetic field-assisted hyperthermia.

Acknowledgements: The European Research Council (ERC-Stg-2016 TSuNAMI: 15-01953S) is gratefully acknowledged. Experiments were supported by the Materials Growth and Measurement Laboratory MGML (see: http://mgml.eu) and NanoEnviCZ (http://www.nanoenvicz.cz/en). We gratefully acknowledge P. Morales, ICMM Madrid and C. Cannas, University Cagliari and their group members for providing samples.

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PL07-T01

EXPLORING MAGNETO-VOLUME ANOMALIES AND MAGNETO-CALORIC EFFECT IN R_2FE_{17} INTERMETALLIC ALLOYS

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ABSTRACT

R_2Fe_{17} compounds (R = rare earth) exhibit a variety of magnetic behaviors (ferro-, antiferro-, or ferri-magnetic and more complex magnetic orderings such as helimagnetism or fan magnetic structures) depending on the rare earth element. Moreover, all of them display large magneto-volume anomalies induced by the strong dependence of the magnetic exchange interaction on the Fe-Fe interatomic distances [2-4]. In addition, these binary intermetallics show a moderate magneto-caloric effect, MCE, with values of the magnetic entropy change, ~ 6 $Jkg^{-1}K^{-1}$ (for $\mu_o \Delta H$ = 5 T) at room temperature (for R = Nd, Pr). In this talk we will show our recent and more interesting investigations on the magneto-volume anomalies and the magneto-caloric effect of R_2Fe_{17} alloys in polycrystalline, nanostructured and rapid quenched samples.

We acknowledge the financial support from MINECO (Spain) and CONACyT (Mexico).

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PL08-T01

SOFT MAGNETIC NANOCRYSTALLINE POWDERS AND NANOCRYSTALLINE/COMPOSITE COMPACTS OBTAINED BY MECHANOSYNTHESIS AND SPARK PLASMA SINTERING

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ABSTRACT

The paper presents a review of our research on the obtaining and characterisation of some soft magnetic powders produced by dry and/or wet mechanical alloying from Ni-Fe-X-Y and Fe-Si systems. For the Ni-Fe-X-Y system the powders were produced at the same composition as the classical alloys Permalloy, Supermalloy, Hipernick and Rhometal [1-6]. The Fe-Si powders were produced at classical composition (4.5 wt%, 6.5 wt%) and at high Si content (10 wt% and 15 wt%) [7, 8]. The powders were obtained by dry and wet milling under argon atmosphere, using benzene as surfactant. In order to study the influence of milling time on the structure, microstructure and magnetic properties of the alloyed powders, different milling time was used ranging from 1 to 40 h. A heat treatment at 350 °C for 4 h in vacuum was performed in order to remove the internal stresses (induced by milling) and to improve the solid-state reaction of the new synthesized phase. The nanocrystalline/composite compacts were obtained by spark plasma sintering technique from nanocrystalline powders and carbonyl iron or nanocrystalline Fe-Si/Ni_3Fe powders [8, 9, 10]. The powders and sintered compacts were investigated by X-ray diffraction, SEM+EDX, DSC, TG, IR, mass spectrometry, Mössbauer, magnetic measurements (M(T), M(H), B(H)). The alloys were obtained after 2 and 6 hours of milling and annealing at 350 °C/4h for Ni_3Fe, Supermalloy and Hipernick alloy respectively. The crystallite mean size was estimated at 12-14 ± 2 nm, depending of alloy and of milling time. The magnetization measurements at 300 K in magnetic fields up to 8 T showed a continuous decrease of the spontaneous magnetization with increasing milling time. In Fe-10wt% Si powders the heat treatment leads to the formation of the Fe_3Si compound with DO3-type superstructure for low milling times. During the sintering process an interface corresponding to Rhometal alloy composition was created between iron and Supermalloy particles. This leads to an increase of the electrical resistivity and coercivity of the compacts.

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PL09-T03

MICROMAGNETISM, MAGNETIC MICROSTRUCTURE AND THEIR MAGNETO-OPTICAL ANALYSIS

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ABSTRACT

The characterization of magnetic materials in research and development usually relies on the measurement of hysteresis curves, which are determined by the magnetic microstructure of the material. The knowledge of magnetic domains and their substructures is therefore essential for the interpretation of magnetization curves.
Magneto-optical microscopy, in particular Kerr microscopy, is just one among many techniques to image domains and processes, and it may be considered a „classical“ method (compared to „modern“ magnetic microscopy based, for instance, on circular X-ray dichroism or spin-polarized tunneling). Nevertheless, it is the most flexible and versatile technique and due to substantial technical progress in recent time magneto-optical domain imagine becomes very powerful again.
In this presentation, a review will be given on the possibilities and recent developments of magnetic domain imaging by wide-field magneto-optical microscopy. Besides some basics, this includes depth-sensitive and time-resolved domain imaging, a mathematical deconvolution method to enhance the lateral resolution, and on the other hand an overview imaging tool to maximize the field of view. Novel light-emitting diode (LED) lamps allow for contrast separation and enhancement, vector magnetometry and in-situ quantitative Kerr microscopy of complete magnetization processes, as will be demonstrated on magnetic film and bulk materials. By using magneto-optic indicator films (MOIF) with perpendicular or in-plane anisotropy, it is possible to image magnetic poles by Faraday microscopy. With the MOIF technique domain information can be obtained in cases where the sample surface is coated like on electrical steel. By using perpendicular MOIF films the domain contrast is even strong enough to allow for single-shot time-resolved imaging of coated transformer steel up to power frequencies. MOIF films also provide the potential to investigate the role of grain boundaries for flux propagation in such material.

PL10-T03

MAGNETIC ANISOTROPY AND COUPLING IN FE-BASED LAYERED NANOSTRUCTURES

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ABSTRACT

Nanostructured magnetic materials in the form of ultrathin films and multilayers are of high
interest when presenting aspects such as perpendicular magnetic anisotropy (PMA) and ferromagnetic/antiferromagnetic (FM/AF) coupled interfaces due to their potential for applications in spintronic devices, but many effects in these kind of systems still need better understanding. In such types of layered magnetic nanostructures, the possibility of conducting depth-resolved measurements and accessing buried magnetic interfaces can be important, although challenging. In this talk, studies on the structure and magnetism of layered Fe-Co-based nanostructures grown by molecular beam epitaxy (MBE), and by magnetron sputtering will be addressed. Also the potential offered by the application of isotope-selective measurements for depth-resolved studies of Fe-based layered magnetic systems- thecombination of conversion electron Mössbauer spectroscopy with 57Fe probe layers – will beillustrated. In this talk, I will discussed the influence of chemical order on the magnetic anisotropy of epitaxial Fe/Co ultrathin films grown on a $Cu_3Au(001)$ substrate, the effect of the preparation conditions on the PMA in Pt/Fe-Co multilayers grown by magnetron sputtering, evidencing a magneto-crystalline origin of the observed perpendicular anisotropy, and investigations of depth-dependent spin structure, magnetization reversal and interface interdiffusion in exchange-biased (FM/AF) bilayers. If time allows, other recent studies of layered magnetic systems conducted in our group will be also presented.

Financial support from the Brazilian agencies CNPq, CAPES and FAPEMIG is gratefully acknowledged.

PL11-T03

MAGNETO-RAMAN SPECTROSCOPY-A GREAT TOOL FOR STUDYING THE COUPLING OF MAGNETIC EXCITATIONS TO PHONONS

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ABSTRACT

The Raman spectroscopy is routinely known as a probe of the vibrational states in condensed matter. In magnetic materials, various excitations such as magnons through their resonance with phonons or extremely small changes of local symmetries due to magnetic ordering can be investigated. Recently, the magnetism of carbon nanostructures is frequently discussed. In many cases the phenomena is studied on bulk samples using volume methods such as the SQUID magnetometry. However, these experiments can be strongly affected by contamination due to magnetic impurities, which is extremely difficult to exclude and disentangle. On the other hand the studies of individual carbon nanostructures by the bulk methods is extremely challenging because of low signals, which are barely measurable. Here in this study we combined the *in situ* magneto-Raman spectroscopy to study single wall carbon nanotubes and single-layer graphene grown by chemical vapor deposition. While no significant effects of magnetic fields on carbon nanotubes have been observed, the Raman response of graphene was strongly affected by the applied magnetic field due to the intrinsic magneto-phonon resonances. We will also present several examples of magneto-Raman studies obtained recently in our lab, i.e. spin state switching in spin-crossover molecules.

Acknowledgements: The European Research Council and Czech Science Foundation (ERC-Stg-2016 TSuNAMI,15-01953S and 18-20357S) are gratefully acknowledged. Experiments were performed in the Materials Growth and Measurement Laboratory MGML (see: http://mgml.eu).

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PL12-T04

CHARGE, SPIN AND HEAT CURRENT IN MAGNETIC TUNNEL JUNCTIONS

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ABSTRACT

In the emerging fields of spintronics, spin-orbitronics and antiferromagnetic spintronics, both degrees of liberty of electron, charge and spin, are used and their current can be manipulated and even interchanged. A proper definition of charge and spin currents are described and some calculations for the charge current are performed in magnetic junctions with a ferromagnetic leads (spintronics) and antiferromagnetic (AFM) junctions with a nonmagnetic leads. We show that even in the absence of spin orbit coupling, AFM junction can lead to a detectable anisotropic magnetoresistance due to the structural anisotropy. As a charge current is accompanied by a heat current, where we also investigate the figure of merit ZT in such junctions.

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PL13-T04

FIRST-PRINCIPLES CALCULATIONS FOR ALLOYED CEMENTITE (FE–NI-CR)3C

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ABSTRACT

Cementite, which exists as a disperse phase in carbon steels, strongly affects their mechanical and magnetic properties. Doping elements of steel can also enter the cementite lattice, thus changing the size, shape, and properties of the cementite particles and of the steel also. In particular, nickel, which in itself is not a carbide-forming element, when using in a steel to improve its mechanical properties, was shown to enter the cementite lattice as an iron-substituting element and to change its magnetic properties [1]. In [2-4], cementite with nickel or/and chromium was obtained by mechanical alloying and subsequent thorough annealing. Mechanical alloying allows one to produce nonequilibrium metastable compounds, in particular to obtain samples with a high content of cementite (up to 95–100% [3]). The samples with 0 - 20 % of iron replaced by Ni/Cr were studied in [2-4] by X-ray diffraction, magnetic measurements, and Mössbauer spectroscopy.
In this work, we have performed first-principles calculations of electron structure of cementite with Ni and Cr replacing iron atoms with concentration close to that in [2-4], to acquire additional information on local structure of samples and hyperfine parameters. The unit cells were fully relaxed through finding the minimum of total energy over the lattice parameters and atomic positions. The obtained data for magnetization, atomic magnetic moments, and parameters of hyperfine interaction at Fe nuclei are compared with those for pure cementite and used to interpret experimental magnetic and Mössbauer data.

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PL14-T01
MAGNETISM AND MAGNETO-OPTICAL EFFECTS IN RARE-EARTH BASED AMORPHOUS-LIKE COMPOUNDS

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ABSTRACT

Two different classes of eare-earth (RE) based amorphous-like compounds presenting interesting magnetic and magneto-optical effects will be emphasised. The first one consists in aluminophosphate glasses doped with non-magnetic (La) and magnetic (Dy) RE ions, as obtained by a wet nonconventional methos followed by melting-quenching procedures. The relationship between magnetism and magneto-optical effects in such glasses is discussed starting from the linear dependence of the Verdet constant and the magnetic susceptibility, with a proportionality constant depending on the type of the vitreous matrix and the doping ion. The diamagnetic and paramagnetic contributions to the Faraday rotation are separately investigated and specific compositions for optimal active and passive magneto-optical elements are proposed.The second class consists of Fe-RE based amorphous intermetallics, as ribbons and thin films. The coupling of RE and Fe atoms leading to specific magnetic non-colinear structures, and hence to surprising magneto-functionalities, is dictated by both the RE-RE, Fe-Fe and RE-Fe interactions and by the single ion anisotropy (to be tuned via the type of the RE). In the particular case of amorphous Fe-Dy ribbons (with and without glass forming boron), obtained by induction melting followed by melt spinning procedure, a non-collinear sperimagnetic structure is obtained, which characteristics can be modified through the RE and B content. The structural and atomic configurations were characterized by X-Ray Diffraction (XRD) and Transmission Mössbauer Spectroscopy (TMS) whereas the magneto-strictive effects were evaluated through the changes in the average orientation of the Fe magnetic moment with respect to the sample plane at different temperatures. The case of Fe-Gd and Fe-Dy (Dy is strongly anisotropic as compared to the isotropic Gd) thin films of different concentrations of RE (crossing the compensation point), as prepared by RF-magnetron sputtering with enriched ^{57}Fe will be also detailed. The morpho-structural and compositional characterization was realized via Grazing Incidence X-Ray Diffraction, X-Ray Reflectometry, Transmission Electron Microscopy and Scanning Electron Microscopy coupled with Energy Dispersive X-Ray Spectroscopy. Atomic local configurations and magnetic interactions were studied via Conversion Electron Mössbauer Spectroscopy and Superconducting Quantum Interference Device magnetometry whereas the distribution of local magnetization axis was analyzed via vectorial Magneto-Optic Kerr Effect measurements. A specific magneto-optical behaviour when crossing the compensation points will be also presented and specific peculiarities in magneto-conduction experiments will be discussed. Finally, a specific possibility to investigate magneto-optical effects in such micro-structured RE based systems, with micron-sized Laser spots will be emphasised.

PL15-T01

GRAPHENE SYNTHESIS VIA PLASMA ENHANCED CVD AND MAGNETIC INDUCTION

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ABSTRACT

Since the discovery of graphene in 2004, its unconventional two-dimensional (2D) electron gas properties and outstanding electrical, mechanical, and chemical properties have attracted remarkable interest in condensed matter physics and material science. This opened the way to a large variety of commercial applications including flexible transparent electrodes for displays and photovoltaics,fuel cells, membranes for water purification and desalination. For such applications, the integration of graphene necessitates cost-effective large-area production by scalable processes. Due to its practicality and scalability, chemical vapor deposition (CVD) has become the most common method for graphene synthesis. In parallel, since graphene fabrication uses transition metal such as Cu, Co or Ni, acting as catalysts, large scale heating of metals is routinely done via magnetic induction with fast heating and cooling (typically 30 °C/s) allowing for better control of graphene growth. For these reasons, we developed at LSPM two strategies for graphene synthesis. The first is based on magnetig induction heating using radio frequency (RF) and the second uses microwave plasma enhanced chemical vapor deposition (PECVD). The graphene is grown by decomposition of a carbon source mixed with hydrogen at moderate pressures over polycrystalline metal catalysts. Various carbon feedstock sources have been successfully used to grow graphene including solids such as spin-coated polymethylmethacrylate (PMMA), liquid hydrocarbons such as biomass or more conventional gaseous hydrocarbons such as methane. Regardless of the carbon feedstock, molecular hydrogen H_2 is often added during catalyst annealing to reduce native metal oxide film covering catalyst surface as well as for graphene nucleation and growth. Reaction chambers are made of quartz, allowing in situ optical measurements. We have demonstrated the growth of high-quality graphene films using either inductive heating, where the RF field directly heats the catalytic copper substrate or via plasma enanced CVD over cobalt or copper substrates. The advantages of each process will be discussed on the light of in situ and ex situ measurements. To explore further aspects prevailing in these reactors and to take chemical and energetic effects into account, different computational models were also developed to estimate temerature ans species distribution in these reactors during specific graphene growth conditions.

Keywords: graphene, magnetic induction, microwave plasma, CVD, modeling

PL16-T01

MAGNETIC NANOPARTICLE-MEDIATED THERMAL THERAPIES: QUANTITATIVE COMPARISON OF HEAT GENERATION, THERAPEUTIC EFFICIENCY AND LIMITATIONS

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ABSTRACT

Thermal nanotherapies as magnetic hyperthermia (MHT) and photothermal therapy (PTT) are two promising emergent treatments and non-invasive approaches for tumor ablation, where localized heat generation is mediated by magnetic and photo-activatable nanomaterials [1,2]. Until very recently, these thermal nanotherapies, have been developed separately: MHT is mainly focused on the use of magnetic iron oxide nanoparticles due to their excellent biodegradability, while metallic nanoparticles such as gold nanomaterials are often preferred due to their strong absorption cross sections. They have recently begun to intersect due to the recent discovery and use of photothermal properties of iron oxide nanostructures [3] or to the use of magneto-photothermal hybrids [4], which efficiently combine both heating features in one-single object. A comprehensive comparison of the heating efficiency of magneto- versus photo-thermal effect is presented, where different magnetic nanoparticles have been confronted (iron oxides, cobalt ferrite, spheres, cubes, flowers) with different metallic nanoparticles in aqueous, cellular, and tumoral environment [5]. Intracellular processing markedly impacted MHT, while endosomal sequestration could have a positive effect for PTT. In the search for the most therapeutically viable modality, the effect of nanoparticle concentration and the experimental exposure parameters (magnetic field strengths/frequencies and laser power densities) have been investigated.

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PL17-T03

DZYALOSHINSKII-MORIYA INTERACTION IN ULTRATHIN MAGNETIC STACKS: A ROUTE TOWARD FUTURE SPINTRONIC

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Interesting phenomena in magnetic materials arise from the exchange interaction which plays an important role in magnetism. Indeed, the interaction between electrons originated from Coulomb interaction is mostly responsible for the magnetic behaviour in materials. This interaction is described by a symmetric term, commonly known as the Heisenberg interaction and an asymmetric term referred as the Dzyaloshinskii-Moriya interaction (DMI). Interface DMI (iDMI) has attracted numerous studies because of its ability to generate a new way to store information through various magnetization structures at nanoscale creating and stabilizing magnetic skyrmions. It can change the static and dynamic properties of domain walls (DW) and leads to non-reciprocity of spin waves (SW) having the same wavelength and propagating along two opposite directions through a magnetic material, resulting in a frequency difference. In thin ferromagnetic films (FM), iDMI can appear when the FM is in contact with a heavy metal possessing a strong spin-orbit coupling. iDMI is usually characterized by its effective (D_{eff}) or surface (D_S) constants. It is thus important for both applications and fundamental researches to determine precisely the sign and the value of the iDMI constant. Today, the most direct method for iDMI characterization remains Brillouin light scattering (BLS) spectroscopy where iDMI constant determination is simply reduced to a frequency difference measurement. I will focus on recent results demonstrating efficiency of BLS spectroscopy for the study of iDMi in magnetic stacks.

PL18-T03

Magnetic and magnetocaloric properties of RM_2 Laves phases compounds (R = Er, Tb, Ho and M = Fe, Co, Mn)

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ABSTRACT

RT_2 type intermetallic compounds (where R = rare earth, T=transition metal) have been intensively studied for more than 3 decades for their distinct and complex magnetic behaviors. These materials have taken a special interest in the research of new magnetic devices for application in magnetic refrigeration based on the magnetocaloric effect. The interesting magnetic performances of such compounds are due to the combination of the complementary characteristics of 3d itinerant and 4f localized magnetism. In this work, magnetic and magnetocaloric effect (MCE) properties of the $R(Fe_{0.125}Co_{0.875})_2$ Laves phases compounds (R=Er, Tb and Ho) have been investigated. X-ray diffraction (XRD) analysis revealed that these compounds crystallize in the C15 type Laves phase structure, with *Fd-3m* Space Group. The magnetization curves indicate a ferrimagnetic-ordering induced by computational interactions between the magnetic moments of the rare-earth and those of transition element. The transition temperature (T_C) was determined using the dM/dT curves and was found to be 245K for $Er(Fe_{0.125}Co_{0.875})_2$, 270K for $Ho(Fe_{0.125}Co_{0.875})_2$ and 410K for $Tb(Fe_{0.125}Co_{0.875})_2$. MCE was calculated according to the Maxwell relation based on isothermal magnetization measurements. A maximum value of magnetic entropy change ($-\Delta S_M$) under a magnetic applied field of 5T was found to be 2.7 $Jkg^{-1}K^{-1}$ for $Er(Fe_{0.125}Co_{0.875})_2$. We studied also the substitution effect of iron and manganese by cobalt on the magnetic and magnetocaloric properties of $Er((Fe_{0.8}Co_{x+y}Mn_{0.2-y})_2$ and finally we studied the effect of the substitution in the rare-earth site of the $RR'(Fe_{0.125}Co_{0.875})_2$ with R= Er, Ho and R'=Tb and Gd.

Keywords: Intermetallic, X-Ray diffraction, Magnetization, Magnetocaloric effect.

PL19-T05

SELECTIVE MAGNETIC SEPARATION FOR SEWAGE AND DESALINATION

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ABSTRACT

Water is one of the most important substances on earth. All plants and animals must have water to survive. If there is no water there would be no life on earth. It covers about 71% of the Earth's surface, and is vital for all known forms of life. But only 2.5% of the Earth's water is fresh water. Rapid urbanization and industrialization releases enormous volumes of wastewater, which is increasingly utilized as a valuable resource for irrigation in urban and peri-urban agriculture after an adequate treatment. Urbanization and industrialization drive significant economic activity, support countless livelihoods particularly those of poor farmers, and substantially changes the water quality of natural water bodies. Due to industrialization and urbanization, water resource is becoming more polluted, and risk of this polluted water consumption and its sanitation problem is increasing day by day in most of the developing countries. This growing problem of water scarcity has significant negative influence on economic development, human livelihoods, and environmental quality throughout the world. Hence it has become an essential need for today's environment to protect water from getting polluted or to develop cost effective remedial method for its protection. The technology presented in this paper is based on the capture of heavy metal and other critical elements by means of composite zeolite/magnetic particles, followed by a selective magnetic separation process and combined used of pulsed electrophoresis and magnetic field for the adsorbent regeneration and reuse. The proposed process would be a breakthrough technology for a high-efficiency removal of heavy metal from wastewaters in order to favor the water re-use for agricultural and food production scopes, with the side result to recover metal dissolved. The whole process would allow reducing treatment costs of one order of magnitude, thus fostering its industrial scale implementation. The basic target is the sustainable development of a technology able to provide capture, separation and storage of heavy metals and other critical pollutants, such as As, Cd, Cr, Pb, Tl etc., from wastewater,by a selective magnetic separation technology, in order to re-qualify this important resource for irrigation in urban and peri-urban agriculture. The method is based on production of a composite material consisting of soft magnetic powder coated by zeolite, exploiting both the selective capture of heavy metals on zeolite surfaces and the magnetic properties of magnetic powder for separation of the particles from wastewater after pollutants capture. A variety of zeolites and soft magnetic powders may be used with superparamagnetic properties to avoid agglomeration. After these zeolite shell & magnetic core particles are set in the solution where the critical elements are dissolved, the pollutants are capturedboth by electronic bonds with the zeolite and physical adsorptiononto zeolite surfaces. The heavier the metal ions, the stronger the bond with the zeolite, due to the increasing number of interacting electrons. The selective design of zeolites with adjustable molecular holes, as well as magnetic materials with adjustable magnetic moment is another objective of the project. Thus, different critical elements can be captured, allowing for their selective magnetic separation, and their consequent selection in different tanks by means of simultaneous electrophoresis and pulsed magnetic field. It is worth highlighting that the recovered heavy metals can be potentially commercialized.

PL20-T05

MICROSTRUCTURE AND MAGNETIC PROPERTIES OF FENI AND FESI ALLOYS USING ADDITIVE MANUFACTURING PROCESS

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ABSTRACT

FeNi and FeSi soft magnetic materials are of prime importance in today's magnetic materials research due to their extraordinary magnetic, mechanical and electrical characteristics. Over the past decades, FeNi, FeSi and other soft magnetic materials have been widely investigated for applications in magnetic devices, such as sensors, transformers, inductive devices, electric motors, etc.. However, the consolidation of magnetic system from two or three types of powders to bulk forming components preserving magnetism has always been a challenge. Conventional powder metallurgy techniques such as high-temperature sintering and thermal spraying may lead to a loss of magnetic properties due to the excessive grain growth under high temperature conditions. On the other hand, there is a big difficulty to obtain a precise component elaborated by the conventional methods using magnetic powder. Accordingly, it is necessary to use a post-treatment method in order to develop magnetic bulk materials. Additive Manufacturing (AM) particularly, Selective laser melting (SLM), as a typical solid freeform fabrication (SFF) process, enables the quick production of complex shaped three-dimensional (3D) parts directly from metal powder. The SLM process creates parts in a layer-by-layer way by selectively melting and consolidation of thin layer of the powder with a scanning laser beam. The SLM, due to the flexibility of feedstock and shapes, can be used for producing complex shaped parts, which can not be realized by other conventional methods. Furthermore, in-situ synthesize with layer addition way could decrease the magnetocrystalline anisotropy of material. The extremely rapid melting/cooling process during SLM leads to a fine grain microstructure. Thus, SLM technology has a great potential to elaborate complex parts with promising magnetic properties. In this work, SLM of the FeNi and FeSi mixed powders is performed to prepare magnetic alloys. The microstructural features of these alloys under different laser processing parameters were characterized and discussed.

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ORAL PRESENTATIONS

O01-T04

FIRST-PRINCIPLES PREDICTION OF LATTICE DYNAMICS AND THERMAL PROPERTIES OF ROCKSALT HALF-METALLIC FERROMAGNETS: CASE OF NAO AND KO

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ABSTRACT

Half-metallic ferromagnets (HMF), where one of the two spin channels is metallic while the other shows an energy gap around the Fermi level, are expected to be excellent candidates for technological application in the newly emerging fields of spintronics, spin filtering, digital information processing and storage devices. Using the plane wave pseudopotential approach to density functional theory [1,2] within the generalized gradient and local density approximations (PBE-GGA [3] and PZ-LDA [4]) for the exchange and correlation potential, as implemented in the Quantum Espresso package [5], we investigated the electronic structure and the magnetic properties of sodium and potassium oxides NaO and KO in the rocksalt structure.The phonon frequencies were calculated within the framework of density functional perturbation theory (DFPT) [6] using PBE-GGA. The quasiharmonic approximation [7] allowed us to calculate the evolution with temperature of some fundamental thermodynamic properties such as heat capacity, vibrational entropy, internal energy, free energy of vibration and mean squared displacement.

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O02-T04

DYNAMICS OF MAGNETIZATION IN THE ASSEMBLIES OF FERROMAGNETICNANOPARTICLES: EFFECT OF INTERACTIONS

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ABSTRACT

In recent years, scientists are attracted by ferromagnetic nanoparticles and their potential applications especially in the field of high density magnetic recording. In such nanoparticles, and thanks to their nanometer size, we can reach storage density in the range of 1Tbit/in². However, two problems arise: Superparamagnetic phenomenon due to the nanometer size and the nanoparticle becomes unstable because its magnetization flips with a relaxation time following the Arrhenuis law $\tau = \tau_0 e^{\frac{KV}{k_B T}}$ Dipolar interactions cannot be neglected because of the small distance between the nanoparticles. Several numerical, theoretical and experimental models have been proposed in order to understand the dipolar interactions effect, but sometimes they lead to contradictory results.Our model aims to explain the origin of these contradictions by studying the dipolar interactions effect on ac-susceptibility using the Monte Carlo technique.

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O03-T04

ELECTRONIC AND MAGNETIC PROPERTIES OF MN DOPED ZNO USING THE FP-LAPW APPROXIMATION

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ABSTRACT

We report on the results of the structural, electronic and magnetic properties of ZnO (1 × 1 × 1), (1×2 × 2) in the zincblende (ZB) and rocksalt (RS) phases produced by doping Mn in ZnO structures, considering, for the magnetic interaction between the Mn atoms, both the near and far positions. These are evaluated using density functional theory (DFT).The band gaps of the ZnO semiconductor are calculated by the full potential linearized augmented plane wave (FP-LAPW) method with the local spin density approximation(LSDA) and the modified Becke–Johson (mBJ) potential. The results of the theoretical calculations are compared to the experimental values. The gaps of RS-ZnO are 0.735 LDA eV and 2.688LDA+mBJ eV. They are comparable to 2.45 [1] eV; in the zincblende phase, the gaps are 0.694 LDA eV and 2.946 LDA+mBJ eV compared to the 3.27 [2] eV experimental value. Both the band gap and the total magnetic moment of Mn doped ZnO increased in the supercell (1×2 × 2) for the RS and ZB phases. Our analysis revealed that the mBJ potential is very efficient for the determination of the band gaps of ZnO semiconductors; it is clear that the mBJ potential gives good results for the treatment of the d-orbitals.

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O04-T02
MICROSTRUCTURE AND MAGNETIC PROPERTIES OF $(Fe_{0.6}Al_{0.4})_{100-X}Si_X$ NANOCRYSTALLINE POWDERS: EFFECT OF SILICON ADDITION

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ABSTRACT

$(Fe_{0.6}Al_{0.4})_{100-x}Si_x$ nanostructured alloys with x=0, 5, 10, 15 and 20 at. % were elaborated by mechanical alloying process for a fixed milling time of 72 h. the effect of silicon content on the microstructure and magnetic properties of these alloys was investigated. The X-ray diffraction results reveal the presence, for all samples, of a single (bcc) phase with a lattice parameter which decreases as the Si content increases. The average crystallite size, <D> (nm), follows a exponential decreasing which is more significant after the addition of a low quantity of the Si (5at.%). Indeed, its value falls from 27.5(1) nm for the binary alloy to 10(0.5) nm for the alloy with x=15, and then remains almost constant when Si content further increases to 20 at.%. Moreover, the volume fraction of the grain boundaries (fgb) and the dislocation density (ρ) increase with increasing the Si content up to 15at% and then remain unchanged. Mössbauer spectra show the presence of a sextet (ferromagnetic phase) and a singlet or doublet (non magnetic phase), except for the sample corresponding to x = 10, where the spectrum presents only one singlet. The saturation magnetization, Ms, exhibits a similar trend as the one of <D>, whereas the coercivity decreases to a minimum value corresponding to the sample with x=15%, then increases again to reach a similar value of the sample with x=5%. All the presented results will be correlated and discussed.

Keywords: FeAlSi alloys, mechanical alloying, nanostructured powders, X-ray diffraction, Mössbauer effect, magnetic properties.

O05-T02

MICROSTRUCTURAL AND MAGNETIC PROPERTIES OF ZINC FERRITE AND ANNEALED ZINC FERRITE NANOPARTICLES BY MEANS OF X-RAY DIFFRACTION AND MÖSSBAUER SPECTROSCOPY

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ABSTRACT

Zinc ferrite nanoparticles are synthesized by hydrothermal synthesis in supercritical water method. Portion of this nanoparticles has been annealed at temperature 400°C during 2 hours. Microstructural investigations have been realized using X-ray diffraction (XRD) and Transmission Electronic Microscopy (TEM). From XRD investigations the presence of single phase structure spinel is evidenced and the mean crystallite sizes of the sample were calculated using Maud procedure. For this, the evaluated grains sizes are around 2.3 nm and 9 nm for zinc ferrite and annealed zinc ferrite, respectively. TEM micrographs show that nanoparticles have uniform size and quasi-spherical shape. The magnetic properties are explored by means of ^{57}Fe Mössbauer spectrometry where the spectra were recorded in the temperature range 4.2K-300 K. There is no evidence for the presence of the Fe^{2+} charge state, confirming the perfect stochiometry of the considering nanoparticle. Mössbauer spectrum recorded at room temperature consists on a doublet component due to the superparamagnetic behaviour whereas at 4.2K a magnetically blocked state is revealed. Mössbauer experiments under applied magnetic field (B=8T) parallel to gamma rays direction depict the existence of ferrimagnetic ordering. Owing to a complexity of obtained spectra, a new refinement model based on the use of hyperfine field distribution correlated with angle distribution has been employed in order to realize a qualitative adjustment for spectra. Then, canting angle is found to increase with decreasing grains sizes.

O06-T01

MICROSTRUCTURE, HYPERFINE AND MAGNETIC PROPERTIES OF NANOSTRUCTURED $(Ni_{75}Fe_{25})_{100-X}Si_X$ ALLOY ELABORATED BY MECHANICAL ALLOYING

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ABSTRACT

The present work deals with the effect of Si content on the physical properties of nanostructured $(Ni_{75}Fe_{25})_{100-x}Si_x$ (x=0, 3.5, 6.5, 9, 12 and 15 at %) powders elaborated by mechanical alloying for a milling time of 96 h. The microstructure, hyperfine and magnetic properties of the powders were investigated, as a function of Si content, by means of X-ray diffraction (XRD), Scaning Electron Microscopy (SEM), Mössbauer Spectroscopy and Vibrating Sample magnetometry (VSM). From XRD spectra, the formation of FCC disordered Ni(Fe, Si) solid solution was evidenced after 96 h. As Si content increases, the lattice parameter and the grains size decreases (from ~28 to 15 nm); while the microstrain level decreases from 0.98% to 0.65%. From SEM micrographs, we showed that powders particles become round in shape and decreases in size with increasing Si content. For all Si content, the adjustment of Mössbauer spectra confirmed the formation of disordered ferromagnetic NiFeSi phase. From hysteresis curves, we have extracted the values of saturation magnetization and coercive field for all powders. The evolution of Ms and Hc as a function of Si content will be discussed.

Keywords: Nanostructured powders, $(Ni_{75}Fe_{25})_{100-x}Si_x$ alloy, Microstructure.

O07-T01

EFFECT OF THE ELABORATION TECHNIQUES AND THE POROSITY OF THE SUBSTRATE ON THE STRUCTURAL AND MAGNETIC PROPERTIES OF FE FILMS DEPOSITED ON AL

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ABSTRACT

Three series of Fe/Al samples were prepared by electrodeposition and evaporation methods. We have used polycrystalline porous and non porous Al substrates. Different times have been used in the elaboration process. X-ray diffraction (XRD) and Vibrating Sample magnetometer (VSM) have been used to study the structural and magnetic properties of these systems. In the VSM, the external magnetic field was applied in different directions in the film plane, and perpendicular to the plane. The Influence of the deposition techniques and the substrate porosity on the physical properties was investigated. All samples show an in-plane magnetic anisotropy, with no preferred orientation on the plane of film. The origins of the behavior of the magnetic parameters, such as the coercive and saturation fields, are studied for the three systems; some theoretical analysis and models are proposed.

Keywords: Fe films, magnetic properties, XRD.

O08-T01

ELABORATION AND CHARACTERIZATION OF NIFE THIN FILMS

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ABSTRACT

We have studied the effect of potential deposition on the structural and magnetic properties of electrodeposited NiFe films. NiFe samples were prepared onto FTO substrates for potentials varying from -1 V to -1.5 V. The crystalline structure and magnetic properties of the elaborated films were characterized by X-ray diffraction (XRD) and vibrating sample magnetometry (VSM). From XRD spectra, we have evidenced the formation of polycrystalline face-centered cubic (FCC) NiFe phase. The grains size decreases with increasing the applied potential. The hysteresis curves show a ferromagnetic behavior of NiFe samples. The relationship between coercivity and magnetic parameters will be discussed.

Keywords: NiFe films; electrodeposition; X-ray diffraction; hysteresis curves.

O09-T04

GIANT MAGNETO-RESISTANCE IN THE COCUCO MAGNETIC JUNCTIONS

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ABSTRACT

Different aspects of transport properties at the nano-scale are investigated with the ab initio electron transport code SMEAGOL[1],which has been specifically designed for magnetic materials and which combines the density functional theory (DFT) and the Keldysh non-equilibrium Green's function (NEGF) formalism to calculate the self-consistent electronic structure. In addition, this code allows us to calculate a general relation between the conductance of a ballistic nano-size junction and its scattering properties. This relation is known as the Landauer- formula and it is at the core of modern transport theory. The DFT part is based on the package SIESTA[2]. All the numerical results are obtained using the PBE paramerization [3] of generalized gradient approximation for the exchange–correlation functional. We use Troullier–Martins [4] pseudopotentials to represent the potentials of the atomic cores.
In this work, we study the geant magnetoresistance ratio (GMR) in Co/Cu/Co magnetic junctions. The effects of thickness of the Cu spacer on the transmission coefficient and the I–V characteristic is investigated. The transport properties are correlated to the electronic properties.

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O10-T04

STRUCTURAL, ELECTRONIC, OPTICAL, AND MAGNETIC PROPERTIES OF CO-DOPED CU2O

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ABSTRACT

We investigate the magnetic properties of Co-doped Cu2O. We studied first the electronic and structural properties of Cu2O using the optimization of the lattice constant which is 4.18 A. The calculated gap is found between 0.825 eV and 1.5 eV, these values are in good agreement with the experimental results. The Co atoms are inserted in Cu2O by means of the density functional theory (DFT) using LSDA, LSDA+U, and LSDA+MBJ approximations in the WIEN2k code, based on the supercell model by setting up 12, 24, and 48 atoms in (1×1×2), (1×2×2), and (2×2×2) supercells respectively with one or two copper atoms being replaced by cobalt atoms. The energy difference between the ferromagnetic and anti-ferromagnetic coupling of the spins located on the substitute Co has been calculated in order to obtain better insights to the magnetic exchange coupling for this particular compound. The studied compound exhibits stable integer magnetic moments of 2 μB and 4 μB when it is doped with 2 atoms of Co. Optical properties have also been worked out. The results obtained in this study demonstrate the importance of the magnetic effect in Cu2O.

O11-T04

THE EFFECT OF GEOMETRIC ANISOTROPY ON TRANSPORT PROPERTIES IN AFM SPINTRONIC JUNCTION BASED ON MNPT CONNECTED TO A NOBLE METAL LEAD

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ABSTRACT

AFM spintronics is a new field that can replace the conventional spintronics due to the zero magnetization. In this work, we perform firstly DFT calculationfor MnPt bulk with different orientations of spin, this show us that the geometric structure has a large effect both in magnetic and electronic properties. These results led us to study transport properties and its behavior according to the different configurations mentioned above on AFM spintronic based junction: Noble metal/ MnPt / Noble metal.

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O12-T04

AB INITIO ELECTRONIC STRUCTURE CALCULATIONS OF HALF-METALLIC FERROMAGNETISM IN DILUTED MAGNETIC SEMICONDUCTORS BASED GETE

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ABSTRACT

In this work, we have investigated the structural, electronic and magnetic properties for **$Ge_{1-x}TM_xTe$ (TM=Mn, Fe)** in the rock-salt (RS) structure for x=0.125, 0.25, 0.50, 0.75, 1. The calculations were performed using the full potential linearized augmented plane wave plus local orbitals method (FP-LAPW+lo) within the framework of the density functional theory and the generalized gradient approximation (GGA). Structural properties are determined from the total energy calculations and results are given for the lattice parameters, bulk moduli and spin magnetic moments. The analysis of band structures and density of states reveals that for x= 0.125 and x=0.25 GeMnTe is a narrow gap semiconductor and GeFeTe is a half-metal while for x= 0.5 and x= 0.75 both alloys present a metallic character. Furthermore, we predict the values of spin exchange splitting energies Δx (d) and Δx (pd) and exchange constants $N_{0\alpha}$ and $N_{0\beta}$.

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O13-T04

ELECTRONIC AND MAGNETIC STUDY OF NEW DILUTED SEMICONDUCTORS

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ABSTRACT

Since the discovery of the carrier-mediated magnetism in Mn-doped GaAs in 1990s, the DMS have received much attention due to their potential in spintronic technology. However, despite four decades of intensive work, challenges remain and materials complexity often hinders theoretical understanding. The origin of magnetic ordering and paths to higher T_C remain strongly debated. The recent discovery of the new II-II-V semiconductors, open an optimistic road forward, and Mn-doped $Ba(Zn,Mn)_2As_2$ which is isostructural to the 122 iron-based superconductors with the tetragonal $ThCr_2Si_2$ (122) structure, was shown to become a high T_C ferromagnet upon hole doping. Firstly, the electronic structure of several II-II-V semiconductors was calculated by using the FP-LAPW/GGA method. Secondly, the Mn-doped II-II-V was investigated in order to induce magnetism. Finally, the magnetic properties of K-codoped in Mn-II-II-V were examined.

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O14-T04

INVESTIGATION OF THE MAGNETIC AND OPTOELECTRONIC PROPERTIES OF THE PEROVSKITE GDRUO$_3$ USING DFT+U WITH SPIN-ORBIT COUPLING

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ABSTRACT

We have investigated the structural, magnetic, and optoelectronic properties of the ortho-perovskite $GdRuO_3$ using thefull-potential linearized augmented plane wave (FP-LAPW) method based on the density functional theory (DFT). The generalized gradient approach (GGA) was used to treat the exchange and correlation potential while the GGA+U was found to correct the deficiencies of the GGA. The Hubbard *U* was taken to be 6 eV (an experimental and theoretical value). Besides, the modified Becke–Johnson (mBJ) exchange potential was also adopted along in combination with the GGA+U approach (mBJ+U) to enhance the description of the electronic structure. The A-type antiferromagnetic phase of the compound $GdRuO_3$ is more stable than the other magnetic phases. The calculated magnetic moments in $GdRuO_3$ were found to emerge especially from the Gd-4f states electrons. The different values semiconductor gap obtained respectively with GGA+U and mBJ+*U* were 1.4269 eV and 2.9039 eV. These values were increased at 3.5355 eV with the investigation of spin–orbit coupling effects (SOC) on the electronic structure. The mBJ+*U*+SOC approximation was also used to calculate the optical properties by determining the complex dielectric function from which are derived the other parameters.

O15-T04

SPIN-POLARIZED STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF DILUTED MAGNETIC SEMICONDUCTORS $Ca_{0.75}TM_{0.25}O$ (TM = FE, CO AND NI) IN THE ROCK SALT (B1) PHASE

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ABSTRACT

The structural, electronic and magnetic properties of the diluted magnetic semiconductors (DMSs) $Ca_{0.75}TM_{0.25}O$ (TM = Fe, Co and Ni) were investigated in the rock salt (B1) phase using the full potential linearized augmented plan wave plus orbital (FP-L/APW+lo) method based on spin-polarized density functional theory (SDFT). The lattice constants, bulk modulii, spin-polarized band structures and total and local densities of states have been computed. We calculated the spin-exchange splitting energies ΔE^c and ΔE^v produced by Fe, Co and Ni-3d states and the results indicate that the effective potential for the minority spin is more attractive than that of the majority spin. The s–d exchange constant $N_0\,\alpha$ (conduction band) and p–d exchange constant $N_0\,\beta$ (valence band) were calculated. The magnetic moment value per Fe, Co and Ni impurity atom is found to be 3.59, 2.59 and 1.59 μB. The hybridization between Ca-p and TM-3d reduces the local magnetic moment of TM and produces small local magnetic moment on the non magnetic Ca and O sites. The Fe, Co and Ni-3d half-filled electrons have been treated as valence electrons and due to their hybridization, the ternary alloys $Ca_{0.75}TM_{0.25}O$ (TM = Fe, Co and Ni) have well defined spin-up and spin-down band structures.

Keywords: Ab-initio calculation; FP-L/APW+lo; Diluted magnetic semiconductors; Magnetic moment.

O16-T04

MAGNETIC EXCHANGE INTERACTION OF MN_2SNTE_4

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ABSTRACT

We calculate the structural, electronic and magnetic properties of Mn_2SnTe_4 using density functional theory and modified Becke–Johnson (TB-mBJ) approach as proposed by Tran and Blaha and coupled with the generalized gradient approximation (GGA). Several magnetic configurations are considered. The results reveal that the Mn_2SnTe_4 has an antiferromagnetic character where Mn(3d) ions have great effect on the magnetic properties, and the I-type antiferromagnetic state is found to be the ground state with a reduced magnetic moment on Mn ion as observed in Mn2SnTe4. The optimized structures and magnetic ground states are in good agreement with available experimental results. The electronic structures of these Mn_2SnTe_4 are obtained at their magnetic ground state. The obtained band gap of Mn_2SnTe_4 is 1.32 eV. The calculated magnetic moment on Mn ion is found to be equal to 4.9 μ_B. In this work, we examined the magnetic properties of Mn_2SnS_4 based on the density functional theory (DFT); we have given particular attention to the case of exchange interactions Jij which favors the antiferromagnetic order. Additionally, in order to compare the overall magnitude of the calculated J_{ij} with the experimental results, the Curie-Weiss temperature θ can be calculated from the exchange constants using the mean-field approximation

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O17-T03

PHYSICOCHEMICAL AND MAGNETIC PROPERTIES OF $FE_{50}CO_{50}$ NANOWIRES ELECTROPLATED IN ALUMINA MEMBRANES

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ABSTRACT

The development of one-dimensional magnetic alloys has taken significant place in the scientific community due to their potential application in the nanotechnology industry. Among these alloys, the FeCo equi-atomic systems show very interesting magnetic characteristics (high saturated magnetization, high permeability…) [1, 2]. Their nanowires shape offers them, among other things, a special feature in connection with the resulting perpendicular anisotropy. In this context, aluminium oxide membranes are particularly suitable for the development of these materials because of their easily adjusted geometric characteristics (diameter, length, etc.) and their physico-chemical properties (chemically inert, good thermal conductivity and resistance to high temperatures) suitable for the electrodeposition process of metal alloys and the annealing treatments often carried out. However, this matrix has a compact barrier layer at the bottom of the pores that forms during the anodizing process and whose thickness depends on the applied potential. This insulating layer prevents electrical contact between the metallic aluminum and the porous layer, which prevents nanowires from electroplating.In this work we present the study of the geometric, structural and magnetic properties of $Fe_{50}Co_{50}$ nanowires electroplated in alumina matrixes. The effect of the annealing treatment has also been studied. The alumina matrixes have been treated by electrochemical process in order to thin the barrier layer. Transversal SEM observations revealed a perforation of the barrier layer with smaller diameter branches having a length of about 800nm. The electroplated $Fe_{50}Co_{50}$ nanowires have the same diameter as the alumina pores but non-homogeneous lengths. Structural analysis by X-ray diffraction (XRD) revealed a centered cubic structure (bcc) of the FeCo alloy and the VSM magnetic measurements showed that the easy magnetization axis is parallel to the wire axis. The annealing treatment at 300°C for 22 hours induced a significant increase in the coercivity (from 546.5 Oe to 909.5 Oe).

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O18-T03

INFLUENCE OF THE THICKNESS ON STRUCTURAL, ELECTRICAL AND MAGNETIC PROPERTIES OF NI FILMS ELECTRODEPOSITED ONTO *N*-Si (100) SUBSTRATES

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ABSTRACT

Ni films have been deposited by pulsed electrodeposition method onto *n*-Si (100) substrates. A series of samples have been elaborated for different deposition times at a fixed deposition potential of 2 V. The as deposited Ni films were characterized by Rutherford backscattering spectroscopy (RBS), X-ray diffraction (XRD), Atomic Force Microscopy (AFM), four point probe method and Vibrating Sample Magnetometry (VSM). The RBS experiments revealed that the Ni thickness ranges from 105 to 710 nm. The XRD results show that all films present a texture along the direction <111>. With increasing Ni thickness, the films become progressively smoother; the *rms* surface roughness decreases to 2.295 nm for the thicker film. When *t* increases, a clear correlation between the behavior of the mean grain size and the electrical resistivity was observed. The coercive field increases with Ni thickness (in the 105 to 675 nm thickness range). The saturation field, the squareness and the anisotropy constants have been studied as a function of the Ni thickness.

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O19-T03

EFFECT OF THE MILLING TIME ON STRUCTURAL AND MAGNETIC PROPERTIES OF $(Fe_{0.7}CO_{0.3})_{95}Si_5$ ALLOY OBTAINED BY MECHANICAL ALLOYING

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ABSTRACT

This work focuses on the elaboration of nanostructured $(Fe_{0.7}Co_{0.3})_{95}Si_5$ as a function of milling time, t, (in the 0-60 h range) powders by mechanical alloying process. The structure, microstructure and magnetic properties of as prepared powders were characterized by X-ray diffraction, scanning electron microscopy and vibrating sample magnetometer (VSM). From X-ray diffraction spectra, we have shown that, after 12 h milling, a centred cubic Fe(Co,Si) solid solution was completely formed with a lattice parameter a=2.86105A° at 24 h. During the milling process, the grains size is reduced to a nanometer scale. The hysteresis loops confirmed the ferromagnetic character of FeCoSi nanostructured powders. We have found that the saturation magnetization, Ms, and the coercivity, Hc increases during the milling and reaches a maximum at 24 h and 12h respectively. All these results will be correlated and discussed.

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O20-T04

LOCALIZED ENERGIES AND STATE DENSITY AT THE ALLOY SURFACE

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ABSTRACT

We applied the modelling and analytical approach to investigate and to understand Dynamic of localized spin wave energies at the ferromagnetic alloy surface system Fe/ Ni. The surface breaks the invariance symmetry in the direction normal to it. Also its dynamic is studied in Heisenberg formalism associate with the matching theory in the approximation of the nearest and next nearest neighbours. The bulk modes are determined, furthermore they are necessary to determine localization phenomenon at the disturbed zone. We also calculate the different physical properties. Furthermore the Rayleigh localized magnons and their associate state densities are determined using the Green functions.This quantity is of great use in experimental physics since it is directly measurable. They are determinate as function of the magnetic exchange integral characterising neighbourhood of the perturbed system and the dimensionless frequencies of incident energies.

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O21-T04

LONG-RANGE ANTIFERROMAGNETSIM IN FE-DOPED $ZNAL_2O_4$: A FIRST-PRINCIPLES STUDY

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ABSTRACT

The effect of doping with Fe atoms on the electronic structure and magnetic properties of $ZnAl_2O_4$ spinel oxide was studied by using the first-principles method. The obtained results show that the Antiferromagnetic state is the most stable state in Fe-doped $ZnAl_2O_4$. Moreover, our results show that long-range antiferromagnetism can be produced in Fe-doped $ZnAl_2O_4$. Densities of states (DOS), charge analysis and magnetic moment are analyzed and discussed in a detailed manner to understand the origin of this behavior.

O22-T04

FIRST-PRINCIPLE PREDICTIONS OF ELECTRONIC PROPERTIES AND HALF-METALLIC FERROMAGNETISM IN VANADIUM-DOPED ROCK-SALT SRO

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ABSTRACT

We have used first principle methods of density functional theory within the full potential linearized augmented plane wave scheme to investigate the electronic and magnetic properties of cubic rock-salt ,SrO doped with vanadium (V) impurity as $Sr_{1-x}V_xO$ at various concentration x = 0.25 , 0.50 and 0.75.We have found that that the ferromagnetic state arrangement of $Sr_{1-x}V_xO$ is more stable compared to the anti-ferromagnetic state configuration.The electronic structures have a half metallic (HM) ferromagnetic behavior for$Sr_{0.75}V_{0.25}O$ and$Sr_{0.5}V_{0.5}O$.This feature results from the metallic and semiconducting natures of majority-spin and minority-spin bands, respectively .The HMF gap decreases with the increasing concentration of vanadium atoms due to the broadening of 3d (V) levelin the gap, and hence the $Sr_{0.25}V_{0.75}O$ becomes metallic ferromagnetic.The $Sr_{0.75}V_{0.25}O$ compound revealed a large HM gap with spin polarization of 100%. The $Sr_{1-x}V_xO$ compound at low concentrations seems a better candidate to explore the half-metallicity for practical spintronic application.

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O23-T01

EFFECT OF FE CONTENT ON THE STRUCTURAL AND MAGNETIC PROPERTIES OF TERNARY $(Ni_{60}Co_{40})_{100-x}Fe_x$ NANOPARTICLES SYNTHESIZED BY HYDROTHERMAL ROUTE

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ABSTRACT

In this work, we investigate the effect of iron content on the structure, morphology and magnetic properties of $(Ni_{60}Co_{40})_{100-x}Fe_x$ powders synthesized by hydrothermal method. Several samples have been elaborated for different Fe content (x=0, 3, 5, 7, 10 and 13.5). The as prepared samples have been characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) and vibrating sample magnetometry (VSM). From XRD spectra, we have shown the presence of a cubic face centered (cfc) phase for all Fe content. The lattice parameter increases with increasing Fe content. The grains size varies with Fe content to reach a minimum value of 32 nm for $(Co_{40}Ni_{60})_{90}Fe_{10}$. From Hysteresis curves, we have extracted the saturation magnetization, Ms, and the coercivity, Hc. We noticed that Ms increases and then decreases as a function of Fe content. The values of Hc vary from 156 Oe to 186 Oe depending on the particles shape. All these results will be correlated and discussed.

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O24-T01

Elaboration of Nickel films by PVD: method and procedure

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ABSTRACT

The Elaboration of magnetic material by magnetron sputtering requires the understanding of the relationship between the magnetic properties of the material to be deposited and the magnetic field created by the magnets of the cathode. The magnetic material can completely disturb or annihilate the field lines above the cathode, which leads to a considerable reduction in the density of the secondary electrons, the motive force of the sputtering, and consequently the sputtering rate and the quality of the material. In this work we present the methodology and the procedure for the elaboration of Nickel thin film by using the PVD frame developed in the research unit- Materials Process Environment of the University of Boumerdes in collaboration with the nuclear research center of Birine .

Mots clefs : Nickel, PVD, Magnetron cathode, magnetic field,

O25-T01

DEPOSITION OF TiO_2/Fe_2O_3 COMPOSITE THIN FILMS BY VACUUM THERMAL EVAPORATION

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ABSTRACT

TiO_2 and TiO_2/Fe_2O_3 composite thin films were prepared by vacuum thermal evaporation method. The substrates were annealed at 400°C for 1 hour. In this study the effect of magnetic iron oxide was studied. Films were characterized by Raman spectroscopy, TiO_2/Fe_2O_3 films were taken at room temperature in the range of 100-850 cm^{-1} indicates that iron atom exhibits two oxidation states Fe (II) and Fe(III) simultaneously. It has been reported that the high thermal expansion coefficients of these materials are useful in reducing the residual stresses of Fe_2TiO_5. Surface morphology of films was investigated by scanning electron microscopy (SEM) which exhibit that TiO_2/Fe_2O_3 deposited films are uniform and compact. Optical and magnetic properties are analyzed and discussed.

Keywords: TiO_2/Fe_2O_3 composites, Magnetic, Vacuum thermal evaporation.

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O26-T01

SYNTHESIS AND CHARACTERIZATION OF MAGNETIC IRON OXIDE/CLAY COMPOSITE AND ITS APPLICATION FOR METHYLENE BLUE REMOVAL

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ABSTRACT

In this work, we prepared a magnetic composite by deposition magnetite particles on surface clay KDD3. Coprecipitation method is a simple and low cost method for preparation Fe_3O_4-KDD3. The prepared composite was characterized by ATG, ATD and was explored for removal Methylene blue. Kinetic studies show the adsorption of MB on the surface of adsorbent could be described by the pseudo-second order model. Also, magnetic separation will be applied on rather than the filtration or centrifugation processes. Therefore, it will have potential applications for removing residual dyes from waste water.

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O27-T01

STRUCTURAL AND MAGNETIC PROPERTIES OF NANOSTRUCTURED $Fe_{60}Al_{40}$ POWDERS PREPARED BY MECHANICAL ALLOYING

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ABSTRACT

The FeAl intermetallic is considered as a potential high-temperature structural material due to its particular physical and mechanical properties, such as high melting point, low density, high thermal conductivity and excellent oxidation resistance [1]. Mechanical deformation is known to induce disorder in completely ordered Fe-Al alloys. This effect produces a strong influence on the magnetic properties of these alloys and may even induce ferromagnetic transition in ordered paramagnetic alloys [2, 3]. In this work nanocrystalline $Fe_{60}Al_{40}$ powders were synthesized by mechanical alloying (MA) from elemental powders mixture of Fe and Al. Mechanical alloying was carried out in a high-energy planetary ball mill (Fritsch pulverisette 7), at room temperature. The powders were MA for 20 hours under argon atmosphere. The characterization was carried out via X-ray diffraction (XRD), scanning electron microscopy (SEM) and vibrating sample magnetometer (VSM). The microstructural parameters (the crystallite size, the mean micro-strain, and the lattice parameters) of the bcc-solid solution Fe(Al) were deduced from XRD data. The experimental results indicate that with increasing milling time, the crystallite size decreased to the nanoscale level, whereas the micro-strain and lattice parameter of the disordered solid solution increased. In addition, the sample showed a hard ferromagnetic behavior (Hc = 150 Oe).

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O28-T03

STRUCTURAL AND MAGNETIC PROPERTIES OF $Fe_{64}Pd_{36}$ DEPOSITED ONTO GLASS AND Si (100) SUBSTRATES

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ABSTRACT

We report on the structural, hyperfine and magnetic properties of $Fe_{64}Pd_{36}$ thin films elaborated by thermal evaporation technique onto Si (100) and glass substrates. The structure and magnetic properties were investigated by by X-ray diffraction, SQUID and convertion electron Mössbauer spectroscopy (CEMS). From XRD spectra, we have shown that all samples present a mixture of bcc and fcc phases. The value of magnetic moment for FePd films deposited onto Si(100) is higher than the one of those deposited onto glass. We believe that this different is due to the effect the surface and interface. The relashionship between structure, hyperfine and magnetic properties will be correlated.

Keywords: FePd films, structure, Mössbauer spectroscopy, magnetic properties.

O29-T03

ANALYSIS OF IMPURITIES OF ND-FE-B MAGNET BY NUCLEAR METHOD AND RECOVERY BY PRECIPITATION CHEMICAL OF ND AND PR RARE EARTHS

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ABSTRACT

The products of the new information and communication technologies (NTIC), whose life often not exceed three years, became consumables to the computer image and other waste that contains neodymium and praseodymium (rare earths); in this field of management, treatment and recycling of waste, we propose the recovery of elements such as neodymium and praseodymium, from the super-magnet Nd-Fe-B, Our study provides a simple process and inexpensive. The implementation scheme of our project consists in a first step in developing a plan of experience that has been made specifically to perform the optimization of operating conditions of the precipitation process. This experimental design was inspired by a statistical technique advanced design of experiments known factorial design. The method begins by embrittlement in liquid nitrogen (-196°C), dissolution in an acidic solution and recovered by a unit operation of chemical engineering, we add an oxalic acid solution to precipitate Nd as neodymium oxalate, followed by purification of neodymium and praseodymium. For characterization we used the following techniques [6]. The neutron radiography, the neutron activation analysis (NAA) and the scanning electron microscope coupled with EDX. The identification of the most intense peaks in the XRD spectrum shows the presence of a single compound which hydrated neodymium oxalate chemical formula $Nd_2(C_2O_4)_3 10H_2O$. The counting of γ spectrum shows that the purity of the precipitate is higher than 99%. Then, the thermal decomposition transforms this powder to neodymium oxide. After the reduction we obtain pure neodymium, the analytical balance shows that this magnet contains 26% of neodymium.

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O30-T03

EFFECT OF LANTHANUM SUBSTITUTION ON COBALT FERRITE STRUCTURAL AND MAGNETIC PROPERTIES

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ABSTRACT

Cobalt ferrite ($CoFe_2O_4$) is a well-known hard magnetic material with high coercivity and moderate magnetization **[1].** This work was focused on the study of the influence of small amount of lanthanum addition (0%, 5% and 10%) on the microstructural and magnetic properties of $CoFe_2O_4$. $CoFe_{2-x}La_xO_4$ powders and sintered samples were prepared by standard ceramic technique. The morphology and the structural properties were investigated by the scanning electron microscope (SEM) and the X-ray diffractometer (XRD). XRD measurements show that the $CoFe_2O_4$ spinel phase was formed after 8 hours of grinding. The magnetic characteristics were studied by vibrating-sample magnetometer (VSM). Preliminary results show that lanthanum has a direct influence on coercive field, Hc, and saturation magnetization, Ms, values, where these parameters increase with the increase of the doping concentration. Furthermore, it seems that the addition of lanthanum small amounts enhances the magnetic properties behaviour of $CoFe_2O_4$.

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O31-T03

ELASTIC MODELING OF SPIN-CROSSOVER NANOCOMPOSITES: TOWARDS MULTI-SPTEP SPIN TRANSITIONS

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ABSTRACT

Spin-crossover (SCO) solids have been studied for their fascinating properties, exhibiting first-order phase transitions and macroscopic bistabilities, accompanied with significant magnetic, structural and optical changes. These exceptional properties make these materials promising for applications as high-density information storage and optical switches. Recently, the important progress made in chemistry allowed the design of spin-crossover nanocomposites, combining the properties of two types of spin-crossover solids having different properties, like different lattice parameters, bulk modulus's, transition temperatures, ligand fields etc. In this work, we examine, using a microscopic electro-elastic description, the thermodynamic properties of such SCO nanocomposite, and look for the physical conditions underlining the emergence of unconventional behaviors, such as two or three steps transitions, as reported very recently in literature.

O32-T05

NUMERICAL ANALYSIS OF INDUCTION HEATING IN A CRYSTAL PULLING-CZ FURNACE

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ABSTRACT

Numerical modelling is conducted to study the induction heating of a crucible for crystal growth. The aim is to accurately determine the thermal field in the central region, to give some important information for better interpretation of the process. All types of heat transfer are considered. The prediction of thermal losses in all parts of furnace is important to overcome. Numerical simulation taking into account physical phenomena is a precise powerful tool, but needs long calculations. Many studies have been reported on modelling of transport processes in crystal growth considering the different involved phenomena. Induction heating is based on Lenz's law. The current in the coil generates an electromagnetic field which induces heat in conductive materials. The computed temperature distribution in the furnace is shown. The buoyancy resulting from density change due to thermal gradient and the Lorentz force are the major driving forces in the melt flow. The rotational part accelerates the fluid in the direction of the magnetic field gradient. This force creates a vortex structure causing the melt at the free surface to flow to the crucible wall, against the natural buoyant convection. We first give a description of the considered crystal growth setup, and then we present the mathematical model used to perform the simulation, and discuss the main results obtained in the case of (semiconductors). The main parameters including the crucible–coil distance, frequency and turns of coil could be optimized in order to reduce the energy consumption, to ensure a controlled melting of the materials.

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O33-T05

MODELLING OF MAGNETIC FORCE AND IDENTIFICATION THE MAGNETO-MECHANICAL PROPERTIES OF ELASTOMER

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ABSTRACT

This paper is devoted to an experimental study of the magneto-mechanical behavior of a magnetorheological elastomer of 20% of the micron-size ferromagnetic particles loading rate and elaborated under the action of a magnetic field. The characterization of the rheological properties and the interaction between the micron size ferromagnetic particles as a function of the intensity of the magnetic field are studied. The results obtained clearly show a high energy dissipation properties of the composite, accentuated by its modified structure from the interaction forces between the particles that are aligned, which gives adjustable viscoelastic structures properties, depending on the volume fraction of particles and the magnetic field intensity.

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O34-T05

PREPARATION, CHARACTERIZATION AND VALORIZATION OF HYDROXIDE FERRIC (III) MODIFIED ALUMINOSILICATE KIESELGUHR MATERIAL

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ABSTRACT

Diatomite-Fe_2O_3 hybrid material honey-comb structure with circular pores synthetized as a heterogeneous catalyst for photodecolourisation of organic contaminants by a novel method. The diatomite has a strong silica content (from 80 % to 90 %) it is a light rock with a variable density from 1 to1.2 for the fresh rock and 0.5 for the dry rock. The importance is to know its structural composition led us to make a study for the physico-chemical characterization and textural of the diatomite by methods of analysis such as x-rays diffraction (XRD), Fourier Transform Infrared spectroscopy (FT-IR), scanning electron microscope (SEM), x-rays fluorescence (XRF),and UV-Vis spectrophotometer. The diatomite which will be modified by iron « the deposit of ferrihydrite on raw diatomite by $FeCl_2.4H_2O$ » and NaOH to increase the specific surface area of this material. The results obtained enabled us to show that the heterogeneous photocatalysis on the TiO_2-deposit mixture of ferrihydrite on raw diatomite and thus effective to eliminate to then dye from industry from textile.

Keywords: Diatomite, Fe_2O_3, photodecolourisation, TiO_2 , ferrihydrite.

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POSTER CONTRIBUTIONS

P01

A NOVEL THEORETICAL DESIGN OF ELECTRONIC STRURTUREAND HALF-METALLIC FERROMAGNETISM IN THE 3d (V)-DOPED ZINC BLENDE ZnS FOR SPINTRONICS USING MBJ APPROXIMATION

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ABSTRACT

In this work, we have investigated the structural, electronic and magnetic properties of vanadium (V) doped zinc sulfide $Zn_{1-x}V_xS$(x = 0.125, 0.25, 0.50 and 0.75) for zinc blende structures in order to search new dilute magnetic semiconductor (DMS). As implemented in WIEN2K code, the full potential linear augmented plan wave FP-LAPW approach within the spin-polarized density functional theory (SPDFT) was the base of first principles calculation in this investigation.

The structural properties are executed using the Wu-Cohen generalized gradient approximation WC-GGA. Moreover, we devoted ourselves and well presented the electronic and magnetic properties by using the modified Becke-Johnson potential combined with the LDA correlation (mBJLDA). Among the various compound studied, we identify one metallic candidate: 75% V-doping of the Zn-sublattice all others compounds have a half-mettalic (HM) ferromagnetic (FM) behavior. Therefore, the $Zn_{1-x}V_xS$ seems to be a new potential candidate for future spintronics applications.

In order to validate the effects resulting from exchange splitting process, we calculated the exchange constants $N_{0\alpha}$ and $N_{0\beta}$. Moreover, for each concentration x, the value of total magnetic moment has been estimated to equal to 3 μ_β except, for $Zn_{0.25}$ $V_{0.75}S$. Furthermore, we found that small local magnetic moments on nonmagnetic Zn and S sites are created and the local magnetic moment of V from their free space charge value of 3 μ_β is reduced through the p-d hybridization.

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P02

HALF METALLIC BEHAVIOR IN VANADIUM DOPED CaS: AN AB INITIO STUDY

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ABSTRACT

Spintronic devices are currently being researched as alternatives to traditional electronics. Spintronic device operation relies on the movement and manipulation of spin-polarized electrons, in which there are three main processes that must be optimized in order to maximize device efficiencies. These spin-related effects are; the injection of spin-polarized electrons, the transport and manipulation of these carriers, and the detection of spin-polarized currents. In this paper electronic structure and half-metallic ferromagnetism of V doped CaS have been studied using the ab-initio method within the DFT framework. Appropriately constructed supercell of 16 atoms along with the full structural optimization of this cell are used for studying the effect of V ions substitution on the magnetism and electronic properties of the CaS compound. Our results reveal that the V ions can induce ferromagnetic ground state in these compounds. V ions substituted CaS exhibit half-metallic behavior, thereby exhibiting 100% spin polarization. We further observed that the electron correlation effects on these materials do not affect the half-metallic ferromagnetism of these compounds. The V substituted CaS compounds are thus an interesting class of half-metallic materials that deserve further studies.

P03

OXIDES FILMS DEPOSITED BY DC MAGNETRON REACTIVE SPUTTERING

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ABSTRACT

Copper oxides films have been successfully deposited onto glass/Si (100) substrates by DC reactive magnetron sputtering in Ar/O_2 gas mixtures, while varying oxygen flow rate. The obtained results based on the structure and magnetic properties are discussed. Depending on the oxygen flow rate, the films reveal different morphologies of Cu_2O, Cu_4O_3 and CuO phases. In addition, the magnetic properties of the copper oxides thin film were investigated by vibrating sample magnetometer (VSM) method. The magnetic properties of copper oxides thin films are strongly influenced by the oxygen flow rate.

Keywords: Copper oxide; sputtering, magnetic properties.

P04

STRUCTURAL AND MECHANICAL PROPERTIES OF THE ANNEALED VANADIUM NITRIDES THIN FILMS

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ABSTRACT

Transition metal nitrides and transition metal carbides have been largely studied for their scientific and technological importance. Among these transition metal based films, vanadium based films, such as, V-C, V-N, V-N-C. For this reason, the influence of different nitrogen and carbon on the structure and mechanical properties of sputtering based vanadium coatings was comprehensively investigated by X. WU et al., S. SHAH [1, 2] and AISSANI et al. [3] studied the microstructure of magnetron sputtered VN and coating with different nitrogen and carbon concentrations. The purpose of this study joins to investigate the thermal treatment effect on the hardness and wear resistance of the VN/XC100 system for different thickness. The films were deposited by RF magnetron sputtering with 10 and 20 %N_2 pressure in the mixture gas (Ar+N_2). The samples were annealed in interval temperature between 800 to 1000 °C since 1 h, it form the vanadium nitrides and carbides. Then the pieces were characterized by X-ray diffraction, (EDS, WDS) and (SEM), the mechanical properties were analyzed by nanoindentation test. The X-ray diffraction analyses point the stability of the VN and V_2N nitrides at 800 °C; they transformed to (V, N) C and (V, N)$_2$C from 1000 °C. The X microanalysis results show the diffusion mechanism between the vanadium film and the steel sample. From the variation of: V, N, C, O elements concentration with the change of annealing temperature. The variation of N_2 percentage between 10 and 20 % show a clear improvement in the adhesion, residual stress and the hardness.

Keywords: Vanadium nitrides; Vanadium carbides; hardness; annealing treatment; diffusion.

P05

FIRST-PRINCIPLES STUDY OF STRUCTRURAL, ELASTIC, ELECTRONIC AND THERMAL PROPRETIES OF THE TERNARY INTERMETALLIC GdTiGe AND GdTiSi

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ABSTRACT

The full-potential linearized augmented plane wave (FP-LAPW) method using the generalized-gradient approximation (GGA) and the local density approximation (LDA) within the framework of density functional theory (DFT) is applied to the study of structural, elastic, electronic and thermal properties of CeScSi-type GdTiGe and CeFeSi-type GdTiSi intermetallic compounds. Elastic constants are calculated to investigate stability criteria and the mechanical nature of the studied materials. Both compounds are found to be mechanically anisotropic, and ductile, and meet the elastic stability criteria. To complete the fundamental characteristics of both compounds, we have analyzed the thermodynamic properties using the quasi-harmonic Debye model. The obtained results are in a favorable agreement with available experimental and theoretical data.

P06

MELT SURFACE TEMPERATURE MONITORING IN TILTABLE INDUCTION FURNACE

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ABSTRACT

The supervision of induction furnace is the subject of increased development because of the increasing demands on reliability and safety. An essential aspect of the pyrometers of induction furnace is the determination of the exactly temperature on the melt surface related to the current and frequency flow resulting from optimum coil position depending on the applied actual power. With the aid of the mathematical model who describe the appearance and development of the temperature change in the area of inductive cold wall crucible melting, estimation and decision methods it is possible to determine the change of temperature variation corresponding to direct visualization of a meniscus forms on the melt surface under the energy created by the induction coil, this last can fully or partly influence of this meniscus. To solve the problem of pyrometer temperature change variation we propose the determination of the total interaction force related to the operating current of the induction generator. To study the this contribution presents an application for temperature melt change detection to through a case study of the tiltable induction furnace with induction generator MFG-20 indicates that the pyrometer of the measurement temperature is powerful device injunction with the development of a new control method.

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P07

ELECTRONIC AND THERMAL TRANSPORT THROUGH Fe/GaAs/Fe JUNCTION

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ABSTRACT

In the context of thermoelectricity, a high figure of merit ZT [1] is achieved either by increasing the electric conductivity and/or decreasing the thermal conductivity. However in most materials both conductivities go side by side. Therefore, a junction consisting of a metalic leads and a semiconducting or insulating spacer is investigated. The high electric conductivity of the metal and the low thermal conductivity of a such spacer is combined in order to reach a high ZT. In this work we investigate the electric conductivity of the Fe/GaAs/Fe magnetic tunnel junction, using the density functional theory and the non-equilibrium Green's function framework as implemented in the SMEAGOL code [2]. We show that the electric conductivity can be tunned by changing the interface termination Ga or As and by changing the thickness of the spacer.

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P08

DETERMINATION OF IRON MAGNETIC MOMENT IN $Fe_{100-x}Pd_x$ (x=15, 20, 36) THIN FILMS

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ABSTRACT

$Fe_{100-x}Pd_x$ thin films alloys (x = 15, 20 and 36 at.%) were deposited by evaporation method onto glass and Si (100) substrates. In order to study the influence of palladium concentration and the substrate, the as-deposited films were characterized by X-ray diffraction (XRD) and conversion electron Mössbauer spectroscopy (CEMS). The relationship between structural and hyperfine properties will be correlated and discussed.

Keywords: FePd films, structure, Mössbauer spectroscopy

P09

GGA+U CALCULATIONS OF ELETRONIC PROPRETIES OF ZnO: Eu^{3+}

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ABSTRACT

Eu^{3+} doped phosphors with charge compensation are potential candidates of red emitting phosphors for lamp applications. Charge compensation improves the luminescence performance of the material. The charge compensation can most probably be achieved by three possible mechanisms: (a) two Zn^{2+} ions are replaced by one Eu^{3+} ions and one monovalent cation, $2Zn^{2+} \rightarrow Eu^{3+} + Li^{+}$, where Li^{+} is acting as a charge compensator; (b) the charge compensation is provided by a zinc vacancy (V_{Zn}) defects, $3Zn^{2+} \rightarrow 2Eu^{3+} + V_{Zn}$, the subscript Zn denotes an ion in a normal zinc site in the lattice; (c) two Zn^{2+} ions are replaced by one Eu^{3+} ions with the presence of interstitial oxygen (Oi), $2Zn^{2+} \rightarrow 2Eu^{3+} + Oi$. Electronic structures of the crystals corresponding to the three models are evaluated by the first-principles quantum mechanical calculations based on the density functional theory. It is found that the charge compensator defects make Eu^{3+} doping in ZnO energetically more favorable. They break the local symmetry around the Eu^{3+} ion and lead to deep states below the empty upper band, the conduction band that could facilitate intra-4f shell transitions, which can obviously improve the emission intensity of Eu^{3+}-doped ZnO. Therefore, the effect of these defects on the host crystals electronic band states relative to the Eu^{3+} states is reported, since both electron transfer and electronically energy transfer processes enhance the performance of optoelectronic devices based on this material. These theoretical insights are helpful for designing rare-earth doped oxide materials with high photoluminescence (PL) performance. The later is based on the full potential linearized augmented plane wave method (FP-LAPW), an approach which is among the most precise and reliable ways to calculate the electronic structure of solids. The generalized gradient approximation (GGA) method was applied to the non-doped material. In order to describe better the strongly correlated 4f electrons of the Eu^{3+} the GGA+U method was used. The GGA+U method requires as the input the Coulomb repulsion strength (Hubbard parameter U) and the exchange parameter J (magnetic coupling constant), which are related to the Slater integrals**.** In this study, the effect of Eu^{3+} doping on lattice parameters, spin polarized electronic band, and density of states (*DOS*) of ZnO: Eu^{3} is presented and analyzed in details.

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P10

MAGNON SCATTERING IN A SINGLE DEFECT OF 1D LEAD

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ABSTRACT

In the present contribution, we investigate the mognon scattering states in 1D lead of atomic chain which contains a single defect atom. To deal with inhomogeneous systems, due to lack of symmetry, we have integrated the phase field matching theory (PFMT) to compute the eigenvalue problem of our system. Additionally, the transmission and reflection probabilities have been used to calculate the coherent scattering and transport of magnons as well as the conductance across the defect junction.

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P11

STRUCTURAL, ELECTRONIC AND MAGNETIC PROPRETIES OF HALF METTALIC MAGNETISM $RbMnO_2$ FROM FIRST PRICIPLES CALCULATIONS

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ABSTRACT

In order to study the structural, electronic and magnetic properties of half-metallic magnetism$RbMnO_2$crystals we have usedthe spin polarized density functional theory calculations.The 3d orbitals of the Mn atoms were treated using the GGA+U approach. The calculated equilibrium structural parameters agree well with the experimental data. Based on the analysis of the spin-polarized band structure and density of states, we predict the half-metallic character of the studied compound, with the minority spin bands result a direct band gap of 3.43eV,and a total magnetic moment of 4.01 μ_B per unit-cell.

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P12

FIRST PRINCIPLE CALCULATIONS OF STRUCTURAL AND ELECTRONIC PROPRETIES OF PdNiHx

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ABSTRACT

Palladium and its alloys, as well as nickel are all permeable to hydrogen and the most widely studied due to their high hydrogen permeability, their chemical compatibility with many hydrocarbon containing gas streams and their theoretically infinite hydrogen selectivity, The density functional theory based full potential linearized augmented plane wave and projector augmented wave methods within the generalized gradient approximation (PBEsol) for the electronic exchange and correlation have been implemented to understand the phenomenon of Hydrogen diffusion in NiPd , with the L_{10} structure of intercalation of hydrogen atoms in its octahedral sites.Densities of valence state, formation and stability of hydrides of the PdNiHn are analyzed and discussed.

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P13

STRUCTURAL, ELECTRONIC AND MAGNETIC PROPRETIES OF NiMnGe HALF HEUSLER COMPOUND

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ABSTRACT

The full potential linear augmented plane wave (FPLAPW) method based on density functional theory (DFT) within the generalized gradient approximation (GGA) is used to investigate the structural, electronic and magnetic properties of half-heusler NiMnGe compound. We have analyzed the structural parameters, total and partial densities of states. The results show that the half-heusler NiMnGe is metallic ferromagnet in GGA treatment.

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P14

PREDICTION ON STRUCTURAL, ELECTRONIC, MAGNETIC, THERMOELECTRIC AND ELASTIC PROPRETIES OF FULL HEUSLER Ru_2VGe

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ABSTRACT

The full potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT) is used to study the structural, electronic, magnetic, elastic and thermoelectric properties of Ru2VGe full Heusler alloy. Exchange and correlations are treated by both the generalized gradient approximation of Perdew, Burke, and Ernzerh (GGA-PBE) and the modified Beck-Johnson (mBJ).The electronic properties exhibit a half-metallic character for this compound with direct band. Elastic properties indicate that this heusler is mechanically stable. Our material is ferromagnetic and the integer value of the total magnetic moment confirms its half metallicity.

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P15

STUDY OF STRUCTURAL, ELECTRONIC AND MAGNETIC PROPRETIES OF Mn SUBSTITUED (ZnS) FROM FIRST PRINCIPLES

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ABSTRACT

Recently, many efforts have been focused to obtaining II-VI dilute magnetic semiconductors (DMS) by doping semiconductors. Among these latter, sulfide based diluted magnetic semiconductors are attracting increasing attention. Zinc sulfide, a less known semiconductor, could be for interest when doped with transition metal elements. We have studied the structural, electronic and magnetic properties of Zinc blend ZnS and Manganese doping $Zn_{(1-x)}Mn_xS$ (with x=0.25). We used density functional theory (DFT) [1] framework as implemented in the projector augmented wave method (CP-PAW) [2]. The generalized gradient approximation (GGA)[3], as well as hybrid functional have been employed for the electronic exchange and correlation effects. The equilibrium structural parameters, density of states (DOS) and magnetic moment are analyzed and discussed.

Keywords: DFT, spintronic, magnetic semiconductors

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P16

X-RAY DIFFRACTION AND MORPHOLOGY OF $Ni_{100-x}Fe_x$ NANOMATERIALS SYNTHESIZED BY HYDROTHERMAL METHOD

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ABSTRACT

The main objectif of this work consists of elaborating a series of $Ni_{100-x}Fe_x$ nanomaterials ($Ni_{90}Fe_{10}$, $Ni_{80}Fe_{20}$, $Ni_{70}Fe_{30}$, $Ni_{60}Fe_{40}$ and $Ni_{50}Fe_{50}$) by hydrothermal method. For the characterization of these nanomaterials, we have associated three experimental techniques which are X-ray diffraction (XRD), scanning electron microscopy (SEM) and Mössbauer spectrometry (MS). We have shown that the lattice parameter increases with increasing Ni content. The grains size decreases with increasing Ni content with a minimum value of 10 nm for 70%Ni. The morphology varies drasticaly with increasing Ni content. The analysis of Mössbauer spectra reveal the presence of different environments.

Keywords: ferromagnetic materials; nanomaterials $Ni_{100-x}Fe_x$, hydrothermal method; X-ray diffraction; scanning electron microscopy; Mössbauer spectroscopy.

P17

DFT STUDY OF THE STRUCTURAL AND MAGNETIC PHASE STABILITY OF Fe_3Al AND Fe_3AlN

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ABSTRACT

DFT calculations were performed for the metal aluminide Fe_3Al and the nitride Fe_3AlN at several lattice parameters in order to obtain the magnetic phase stability and structural properties of these compounds. We show that the structural and magnetic properties of Fe_3Al can be affected by the presence of N. The Fe_3Al and Fe_3AlN are ferromagnetic (FM) with 1.64 μ_B and 1.10 μ_B as the magnetic moment, respectively. The stable structures of the Fe_3Al and Fe_3AlN nitride are DO_3 and E_{21}, respectively. The possibility of nitrogen to be inserted in the DO_3-Fe_3Al is the tetrahedral site. When we consider lower volumes for Fe_3AlN in the E_{21} structure, we observe a transition from non-magnetic to ferromagnetic.

Keywords*:* Iron aluminides based on Fe_3Al; DFT; Magnetic properties; Structural stability; Nitride.

P18

STUDY OF ELECTRONIC, MECHANICAL, MAGNETIC, AND OPTICAL PROPERTIES OF $Mg_{0.75}TM_{0.25}S/Se$ (TM = Fe, Co, Ni): A FIRST PRINCIPLE APPROACH

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ABSTRACT

A systematic study of the magnetism, mechanical, and optical behaviors of $Mg_{0.75}TM_{0.25}S/Se$ (TM = Fe, Co, Ni) DMS alloys was conducted using the full potential linearized augmented plane wave plus local orbital method (FP-LAPW+lo) [1] under the framework of spin polarization density functional theory (SP-DFT) [2] which implemented in using WIEN2k [3] package. The ferromagnetic (FM) and antiferromagnetic (AFM) ground state energy differences and enthalpy of formation scrutinized their dynamical stability in the FM state. The elastic parameters decided their mechanical stability, ductile behavior, and partial ionic and covalent characters. Moreover, the calculated band structures and density of states revealed the type and origin of magnetism in terms of exchange splitting energies and exchange constants. The Fe- and Ni-doped MgS/Se alloys exhibited half-metallic ferromagnetic (HMF) characteristics, while the Co-doped MgS/Se alloy depicted ferromagnetic semiconducting characters. A reduction in the magnetic moments of the transition metals was observed compared with their free space value, which is due to strong *p-d* hybridization. Furthermore, the optical spectrum showed the maximum light absorbed in the visible and in the UV region of the electromagnetic spectrum, which makes them potential candidates for optoelectronic and spintronic device applications.

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P19

AB-INITIO STUDY OF THE ADSORPTION OF THE F, Si AND SiF SPECIES ON Si(001)-P(2x2) SURFACE

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ABSTRACT

The adsorption of SiF molecule on the Si (001) surface have been investigated by means of first-principle calculations based on the DFT approach, using a pseudo-potential method implemented in the SIESTA code and full relaxation of atomic coordinates. Dissociative and non-dissociative adsorption of the molecule SiF on silicon are obtained depending on it's position and orientation with respect to the silicon surface. SiF molecule is found to be chemisorbed on various sites on the Si surface and the most energetically favourable is intrarow configurations, where the SiF molecule forms a bridge between dimers of the same rows. The dissociation of the molecule occurs only in a few orientations with respect to the surface where the Si atom forms a double coordination with the surface and the fluorine atom forms a bond with another surface Si atom.

P20

ETUDE STRUCTURALE ET TRIBOLOGIQUE DES REVETEMENTS MULTICOUCHES Cr / CrN et Cr / CrN / CrAlN DEPOSES PAR PULVERISATION MAGNETRON REACTIVE DC

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ABSTRACT

The characterizations microstructural, morphological and physicochemical of the various multi-layer coatings are essential within the framework of this study, of which the objective is to connect the mechanical properties of these deposits to their macroscopic and microscopic study. In this investigation, physical vapour deposited (PVD) coatings, on a quenched and tempered x38CrMoV8 steel and silicon substrates, namely, Cr/CrN, Cr/ CrN/CrAlN multilayer with a period of μ = 4 with a Cr, bonding layer were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM) coupled with EDS and WDS microanalyses. Wear tests and optical profilometer observation were carried out. The coatings have a columnar structure, Cr/CrN multilayer coating has a denser structure and a smaller grain size that is about 100 nm than the Cr/CrN/CrAlN multilayer, which is greater than 150 nm, the coefficient of friction of Cr/CrN multilayers is lower than that of Cr/CrN/CrAlN.).

P21

A THEORETICAL STUDY OF MAGNETIC PROPERTIES OF SnO_2 WITH OXYGEN VACANCIES

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ABSTRACT

Actually, Tin oxide SnO_2, in his anatase phase, is one of the most interesting materials. Because of its large band gap energy (E_g=3.6eV)[1]. The anatase phase of SnO_2 is tetragonal with coordinates of atoms Sn(0,0,0) and O(0.31,0.31,0.), space group D_{4h} ≡ P42/mnm and cell parameters a=b=4.74Å, c=3.19Å[2]. The centres Sn an O are describe with all electrons basis set. The aim of this investigation is to calculate theoretically at the level of SCF-LCAO-DFT periodic the magnetic properties such as magnetic moment, ferromagnetic and antiferromagnetic energies and the difference between them for SnO_2 rutile with oxygen vacancies (OV). Calculations are released with CRYSTAL09 program[3]. To obtain the optimized magnetic values we must optimized the parameters of calculations (basis set, Hamiltonian, Spinlock …etc.). Creation of (VO) need use of supercell, in this study we chose a supercell of (2x2x2)p how contain 48 atoms ($Sn_{16}O_{32}$). Different positions and concentrations of (VO) are tested; the choice of optimized structure is based on the minimum of vacancy formation energy (E_f) calculated by the relation: $E_{(OV)} = E_{vac} - E_{st} + 1/2EO_2$ [4]. Once done, the total density of state (DOS) are represented[5] and discussed. In addition to that, an analysis of Mulliken population is released. Finally, we compare our results with those obtained by other works.

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P22

FIRST-PRINCIPLES STUDY OF ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES IN SILICON BASED HALF-HEUSLER ALLOYS

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ABSTRACT

The half-Heusler and the full-Heusler alloys with d^0 elements mainly referred to as half-metallic ferromagnets (HMF) still a field of active research [1, 2]. They have attracted great interest due to their possible applications in spintronics. In this work, the electronic structure and magnetic properties of Silicon based half-Heusler alloys, such as SiNaCa, SiNaSr and SiNaBa have been investigated by the first-principles approach based on density functional theory (DFT) and the full-potential linearized augmented plane-wave (FP-LAPW) method using three crystalline structures α, β and γ. We found that the most stable phase for these ternary half-Heusler alloys is the α structure. Our calculation has been carried out within the Perdew-Burke-Ernzerhof (PBE) under generalized gradient approximation (GGA) and the modified Becke-Johnson (mBJ-GGA) for the exchange-correlation energy and potential. As far as we know, it is the first time to research the detailed electronic structure, magnetic, mechanic and thermodynamic properties of Si based half-Heusler alloys. SiNaCa, SiNaSr and SiNaBa compounds were found indirect band-gap compounds, and their calculated half-metallic band gaps using GGA(mBJ-GGA) are respectively 0.28(0.65), 0.40(0.70) and 0.09(0.38) eV. In all the cases ferromagnetic phase is energetically favored with respect to the paramagnetic one in both α and β structures. We also consider the effect of pressure on the half-metallicity of these compounds the α structure and we find that these compounds maintain their half-metallicity under volume compression. It is shown that our calculated structural and magnetic properties are in good agreement with the available theoretical results.
We have also calculate the density of states, elastic moduli and the phonon dispersion relations of these ternary half-Heusler alloys in the α structure. Moreover, we determine phonon dispersions, phonon density of states, thermodynamic properties in these compounds. These properties cause the ternary half-Heusler alloys to be appropriate choices to create useful devices in spintronics.

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P23

EFFECT OF TIN VACANCIES ON THE ELECTRONIC AND MAGNETIC PROPERTIES OF RUTILE SnO_2: AB-INITIO CALCULATIONS

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ABSTRACT

Rutile SnO_2 is widely studied materials with properties such as conductivity, transparency and large band gap (E_g = 3.6 eV) that make them very useful in solar cells, catalysis, spintronic, optically transparent materials, magnetic support for registration and gas sensors. The presence of intrinsic defects were modified the electronic and magnetic properties of bulk SnO_2. Most of ab-initio calculation demonstrated that Sn vacancies were responsible for the magnetic moments in SnO_2. The effect of Sn vacancies (V_{Sn}) on the electronic and magnetic properties of bulk SnO_2 was performed with CRYSTAL09 program, in the framework of the density functional theory DFT at the B3LYP level and effective core pseudopotential (ECP) basis sets. Rutile SnO_2 has a tetragonal structure with space group D_{4h} ≡ P42/mnm. For all calculation, we used supercell (2x2x1)p of 24 atoms with lattice parameters a'=b'=9.474Å and c'=3.186Å. This supercell contains four primitives units cells of bulk SnO_2. The supercell Sn_7O_{16} was constructed by the removing of one Sn ion, which corresponds to the concentrations of 12.5% V_{Sn} vacancy in the bulk SnO_2. The band structures have been obtained with 21 k-points along the appropriate high-symmetry path across the first Brillouin zone for a tetragonal primitive cell. Total and projected density of states to the neighboring to the Sn vacancy (PDOS), Mullikan population and oxidation states are exploited to analyze electronic structure. Our calculation indicate that bulk SnO_2 is non magnetic, but it shows magnetism with a magnetic moment around $4\mu_B$ due to Sn vacancy (V_{Sn}). The presence of tin vacancy produces a short range of ferromagnetic order in the supercell Sn_7O_{16}. The calculated results are compared with the results reported in the literature.

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P24

MAGNETO-TRANSPORT PROPERTIES OF BI-BASED SUPERCONDUCTORS

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ABSTRACT

An analysis of the temperature dependence of resistivity results under magnetic fields is presented for RE doped Bi(Pb)-2212 superconductors. The thermally assisted flux flow (TAAF) theory is used to explain the dissipative behavior, where the $\rho(T,H)$ curves can be described by the Arrhenius equation $\rho(T,H) = \rho_n \exp(-U_0(T,H)/T)$. The temperature and magnetic field dependence of the upper critical field and irreversibility fields are extracted and analyzed.

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P25

MORPHOLOGICAL STUDY OF MAGNETIC NANOGELS BASED XANTHANE

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ABSTRACT

The growing development of nanotechnologies has led to the emergence of innovative materials that are revolutionizing the field of research, including the development of nanocomposite materials that combine the properties of polymeric matrices with those of inorganic nanoparticles, in particular magnetic nanoparticles. In this work, a study of the properties of magnetic nanogels formed based on Xanthan biopolymer (XG) and magnetic nanoparticles (MNP) of iron oxide (Fe_3O_4) was conducted. An emulsion polymerization technique made it possible to obtain magnetic particles coated with polymer in the form of nanogels. The morphology of the magnetic nanogels obtained was mainly studied by transmission electron microscopy (TEM), allowing the determination of the shape, size and uniformity of the particles. The study of nanogels obtained with and without coating has shown the formation of different networks of hydrogels confirming the presence of nanoparticles in different systems. TEM results indicate formation of spherical Fe_3O_4 nanoparticles. MNPs have homogeneous spherical shape with a size ranging from 3 nm to 13 nm in diameter and a narrow size distribution, while the average size of the xanthan coated Fe_3O_4 MNP is 10.44 nm. The coating of the nanoparticles by the polymer is due to the strong interaction between the Fe_3O_4 MNPs and the hydrogel network, confirmed by the size change of the particles before and after the polymer coating. A better morphology of the polymeric crosslinking network has been observed during the coating of the magnetic nanoparticles by the polymer. These results indicate that the magnetic biomaterials obtained have interesting characteristics that can be exploited as nanomaterials for pharmaceutical applications.

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P26

THE EFFECT OF NaOH CONCENTRATION ON THE STRUCTURAL, MICROSTRUCTURAL AND MAGNETIC PROPERTIES OF Co NANOPARTICLES

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ABSTRACT

We have studied the effect of NaOH concentration on the structural, microstructural and magnetic properties of Co nanoparticles synthesized by hydrothermal method. A series of samples for five different concentrations of NaOH (10, 20, 40, 50 and 60g) were prepared. From X-Ray Diffractometry spectra, we have shown the existence of two phases (FCC and HC) with the concentration of FCC phase that increases with increasing NaOH concentration. The lattice parameter increases with NaOH concentration for both phases. The grains size, <D(nm)>, was found to decrease (increase) for FCC (HC) phase with NaOH concentration. Moreover, the values of <D(nm)> are lower than 30 nm indicating the nanometric state of the powders. From SEM micrographs, it was clearly seen that the morphology changes with NaOH concentration. Indeed, for the lowest concentration, the particles present a floral shape. For the intermediate concentration, the floral shape becomes more forked with a leaf like shape. However, for higher concentration, a dendritic shape is clearly seen. Magnetic measurement indicated that the coercivity of Co nanoparticles reached 209.7 Oe for particles with dendritic shape. All these results will be correlated and discussed.

P27

STABILITY, MAGNETIC AND ELECTRONIC PROPERTIES OF Os-DOPED RHODIUM CLUSTERS: A THEORETICAL STUDY

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ABSTRACT

The stability, magnetic and electronic properties of RhnOs (n = 2–12) clusters in their most stable configurations were systematically studied by using density functional theory (DFT) at M06L/aug-cc-pVDZ level [1,2]. Calculation of the second order difference of energies and fragmentation energies exhibited that Rh_3Os, Rh_5Os, Rh_7Os, and Rh_9Os clusters are more stable than any other clusters. The calculated HOMO-LUMO energy gaps of the RhnOs clusters are found to be in the range of 0.018 to 0.299 eV, implying that the metallic behavior can appear in these clusters. Accordingly, the RhnOs clusters can be employed as heterogeneous nanocatalysts in many chemical reactions. The analysis of the magnetic properties of the RhnOs clusters shows that the total magnetic moment per atom of these clusters varies from 0.67 to 1.75 μB/atom. And, the PDOS analysis reveals that the d orbitals play a crucial role for the magnetism of the RhnOs clusters, and the contribution of the s and p orbitals is small.

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P28

STRUCTURE AND MORPHOLOGY OF ELECTRODEPOSITED CoNi THIN FILMS ON FTO SUBSTRATE

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ABSTRACT

$Co_{50}Ni_{50}$ and $Co_{80}Ni_{20}$ films were elaborated by electrodeposition onto FTO substrates using chloride baths. For each CoNi compound, five samples were elaborated for different potentials ranging from -1.6 V to -1.8 V. The structure and morphology of CoNi films were studied using X-ray diffraction (XRD) and Atomic Force Microscopy (AFM). From X-ray diffraction, we have shown the presence of both HCP and FCC phases of CoNi binary alloy with a well pronounced texture along the <100> plane for all samples. For both series of samples, we have found that the crystallite size increases with increasing the applied potential. However, a moderate change in the lattice parameter has been observed with increasing the applied potential. The AFM images shows that the applied potential influences on the morphology and also the surface roughness of CoNi films.

Keywords: CoNi films; electrodeposition; structure; magnetic properties.

P29

EFFECTS OF A NON-SINUSOIDAL POWER SUPPLY ON THE ELECTROMAGNETIC AND MECHANICAL PERFORMANCES OF A LINEAR INDUCTION LAUNCHER

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ABSTRACT

The application consists on the study of a finite element problem, treated under FEMM software (Finit Element Method Magnetics) as well as MATLAB, of a linear induction motor. It is a motor whose operating principle is the same as its rotary counterpart, but having different performances because of the end effects that occur at the input and the output of the primary or the secondary and which alter them considerably [1, 2]. Therefore, this article focuses on the improvement of that linear induction motor, study being established in terms of the evolution of the electromagnetic force applied on the moving load as well as the distribution of the normal component of the magnetic induction along the armature, in the separate cases of a perfect and a real power supply. For this purpose, we have highlighted the degree of influence of the triangulosine PWM throw the characteristic parameters which are the modulation index m and the adjustment coefficient r on one side, and the determination of the adequate initial position of the load in the other side. In this application, a horizontal displacement of the armature is studied for 41 iterations, with a pitch of 3 mm. The mesh of the field of study is as shown in the figure below.

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P30

STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF $\mathbf{TMS_8^{0/\pm}}$ CLUSTERS, $(\mathbf{TM = Sc - Ni})$

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ABSTRACT

The structural, electronic and magnetic properties of neutral and charged $\mathrm{TMS_8^{0/\pm}}$, $(\mathrm{TM = Sc - Ni})$ clusters have been investigated in the framework of the density functional theory, as implemented in the VASP code with the generalised gradient approximation for the exchange and correlation. The calculated vertical detachment energy, adiabatic ionization potential and vertical ionization potential of S_8 cluster are found to be in good agreement with the available experimental data. The impact of doping S_8 of transition-metal (TM) on the atomic structure, stability, magnetic moment, and reactivity is determined through the analysis of the binding energy per atom, electronic charge transfer, and global reactivity indicators like the electronegativity and chemical hardness.

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P31

STRUCTURAL, ELECTRONIC, OPTICAL AND MAGNETIC PROPERTIES OF CaCoSO Single Crystal

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ABSTRACT

The electronic structure and magnetic properties of the half-Heusler alloys CaCoSO were calculated by using the self-consistent full potential linearized augmented plane wave method within the generalized gradient approximation (GGA) for the electronic exchange and correlation. The total energy minimization of the two phases non-magnetic and ferromagnetic indicates that the latter is the most stable one. Densities of valence state, magnetic moment and band structure are analyzed and discussed.

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P32

MAGNETIC AND ELECTRONIC PROPERTIES OF FULL-HEUSLER Cs_2CrGe

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ABSTRACT

The Magnetic and electronic properties of full-Heusler alloys Cs_2CrGe are examined in this study using FP-LAPW method based on density functional theory. Results of our calculations predict that the Hg_2CuTi-type structure is more stable than the Cu_2MnAl-type structure and the ground state of these alloys is ferromagnetic. The total magnetic moment calculated, is an important in conformity with the Slater-Pauling curve for full-heusler alloys. Band structure of Cs_2CrGe shows half metallic in spin-dn for GGA and mBJ-GGA with an important magnetic moment which equal $4\mu_B$ which is in good agreement with the Slater-Pauling rule.

Keywords: *Full-Heusler , Half-metallic ferromagnetic, FP-LAPW method, GGA, mBJ*

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P33

CARACTERIZATION OF PERMALLOY $Ni_{1-x}Fe_X$ ELABORATED BY EVAPORATION UNDER VACUUM

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ABSTRACT

In the present work, we are interested in the structural, morphological and electrical properties of Permalloy (Py) thin films prepared by thermal evaporation and the impact of the thickness on their different properties. For this purpose, a series of Permalloy thin layers of different thicknesses were deposited by vacuum evaporation from a ground powder forming an Fe-Ni alloy of composition 80% Ni and 20% Fe on monocrystalline silicon substrates, with (111) orientation. Analyses were performed using X-ray diffraction (XRD), atomic force microscopy (AFM) and the four-points method. The interpretation of the X-ray diffraction spectra allowed us, among other things, to affirm that the films are poly-crystalline with the coexistence of several textures. Generally, the lattice parameter of Ni1-XFeX (Py) samples is smaller than those of a-bulk. As a result, our samples show a monotonous increase in grain size as the thickness increases. From the observations of the AFM technique, we have established that the layers are smooth or very slightly rough overall. The results of the roughness measurement for our sample series show very low values, and the average roughness (RMS) increases as a function of the thickness, the maximum of which is 13.2 nm, corresponding to a thickness of 600Å. For electrical measurements, there is a monotonous increase in electrical resistivity with the change in thickness, the maximum value, ρ = 27μΩ.cm, corresponding to the thickness of 600 Å.

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P34

SYNTHESES AND CHARACTERIZATION OF Co NANOMATERIAL PREPARED BY HYDROTHERMAL ROUTE

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ABSTRACT

Series of Pure Co nanomaterials with different $CoCl_2,6H_2O$ concentrations were synthesized by hydrothermal route adopting a simplified protocol. Structural and microstructural properties of the powder were investigated by means of X-ray diffraction, scanning electron microscopy (SEM), and energy dispersive X-ray. From X-ray diffraction analysis, we have shown that Co nanomaterials crystallize according to the two allotropic forms: (CFC) and hexagonal (hcp). The purity of our powder was confirmed by EDX analysis. Structural analysis shows a significant reduction of the crystallite size to the nanoscale with a minimum value of the average crystallite size about 10nm for a concentration of 0.5 mol/L. SEM micrographs shows a change in the morphology of particles as a function of the concentration of precursor.

Keywords: Co nanoparticles, hydrothermal, strcuture, morphology

P35

SYSTEMATIC STUDY OF MAGNETIZATION REVERSAL IN SQUARE FE NANODOTS OF VARYING DIMENSIONS IN DIFFERENT ORIENTATIONS

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ABSTRACT

Ferromagnetic nanoparticles can be used for data storage, spintronics, and other applications. Especially vortex states are often suggested to be used to store information. Due to the shape anisotropy dominating in nanoparticles, magnetization reversal processes can be expected to depend not only on the dimensions, but also on the orientation with respect to the external magnetic field [1,2]. While several papers evaluate magnetization dynamics, including vortex precessions, in round nanodots, square nanodots are less often investigated. Here we report on different magnetization reversal processes found in micromagnetic simulations of square Fe nanodots with lateral dimensions between 100 nm and 500 nm and thicknesses between 10 nm and 50 nm. Choosing magnetic field orientations parallel to one of the square edges and under 45°, seven different reversal mechanisms were found, most of them including a single-vortex state, while in some cases two, three or more vortex-antivortex pairs were found. The ground state, i.e. the magnetic state at vanishing external magnetic field, was often a single-vortex state, making the nanodot with the respective dimensions suitable for data storage applications. The stability of this state, i.e. the field range over which it existed, depended strongly on the lateral dimensions and the dot thickness and was largest for small lateral dimensions and large thicknesses.

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P36

INFLUENCE OF DEPOSITION CURRENT DENSITY ON THE ELECTRODEPOSITED TERNARY CoFeCu FILMS

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ABSTRACT

CoFeCu alloys have attracted great interest due to their magnetic and magnetoresistive properties which have potential applications such as data storage devices and magnetoresistive sensors. CoFeCu films were electrodeposited at high pH, from bath containing sodium acetate and their structural and morphological properties were studied. The morphology and elemental composition of the films were determined by scanning electron microscope and energy dispersive X-ray spectroscopy, respectively. The presence of only or two phase structures (FCC (Co) or BCC (Fe)) in the X-ray diffraction patterns of the films is depended to the current density polarization. At low current density polarization (1-5 mA/cm2), the X-ray diffraction patterns showed the formation of two phases Co(FCC (Cu) +BCC (Fe)). Moreover, by increasing current density (10-15 mA/cm^2), the phase structures of the films were changed from (FCC (Co) +BCC (Fe)) to FCC (CoCu). Scanning electron micrographs illustrated that using pH (about 5.2) displayed the micro-voids in the deposited when a current density is increased to15 mA/cm^2.

P37

IMPROVEMENT OF MAGNETIC AND ELECTRICAL PROPERTIES IN (BI,PB)-2234 CERAMICS BY THALLIUM FLUORIDE AND YTTRIUM DOPING

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ABSTRACT

In this study, we have investigated the effect of magnetic field and doping with thallium fluoride TlF_3 and yttrium Y^{3+} on $Bi_{1.8-x}Tl_xPb_{0.35}Sr_2Ca_{3-z}Y_zCu_4O_{12+\delta}F_{3x}$ superconductorswith x = 0, 0.1 and z = 0, 0.2, prepared by solid state reaction method. The analysis of the X-ray diffraction results reveals that all the samples are composed of only Bi-2234, Bi-2223 and Bi-2212 phases. The SEM photographs show randomly distributed grains with a flat shape then the grains of the sample with x = 0.1 and z = 0.2 are more connected than those of the other ones.Resistivity curves indicate an improvement of the transition width(ΔT_c) and the residual resistivity (ρ_0)of the samples asTlF_3 and Y^{3+}content is increased.The activation energy$U_0(H,T)$calculated from the relationship $\rho(H,T)=\rho_0 exp(-U_0\ (H,\ T)/k_BT)$ in the thermally activation flux flow(TAFF) region [1,2] is enhanced with doping which attest of the improvement flux pinning strength into the grains[3].Ac susceptibility measurement$\chi'(\chi'')$ show that the onset temperature of diamagnetismis remained almost constant under applied magnetic field (H =2 and 10 Oe) for all samples suggesting that Tl^{3+},Y^{3+} and F^- substitution do not affect the CuO_2 planes.It was found that the temperature value of the intergranular AC loss peak (T_{pj}) isincreased with TlF_3 and Y^{3+} doping.This behaviour is explained by a strong links between the gains, which is in good agreement with ΔT_c.However, T_{pj}shifts to lower temperature with broadeningas the magneticfield increases [4]. In the real part of$\chi'(\chi'')$ curves it observed that the diamagnetic signal is remained constant with doping, but it was reduced under applied field.

P38

STUDY A MAGNETO-PHOTONIC CRYSTAL STRUCTURE

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ABSTRACT

In this paper Photonic crystals (PCs) have gained significant interest worldwide over the last two decades due to the existence of a band gap PBG, and the ability to control electromagnetic waves, these crystals are structures of which the refractive index varies periodically in one, two or three directions of space, introducing a defect (point or line or both) in these Structures, the periodicity and completeness of the band gap is broken and the propagation light can be located in the PBG region. Non reciprocal photonic devices, including optical isolators and circulators, are indispensable components in optical communications systemsthe goal of integrated magneto-optical (MO) isolators is to incorporate nonreciprocal devices onto photonic platforms in order to achieve the photonic analog of the integrated electrical diode [1]. Electromagnetic wave propagation in periodic media is first studied by Lord Rayleigh in 1888. These structures are One Dimensional (1D) Photonic Crystals (1DPCs) which have a PBG that prohibits the light propagation through the planes [2]. When magneto-optic materials and photonic crystals are combined, new components based on magneto-photonic crystals emerge to exalt the non-reciprocal effects of propagation. As part of this work we use magneto-photonic crystals to design and amelioratetelecommunication device like the ring. The output transmission efficiency of magneto optic and photonic crystal ring resonators are investigated and studied, a 2D ring resonator using magneto optic and photonic crystals in ring lattice with dielectric rods in air configuration was designed and its transmission spectrum studied. The perimeter of the ring in a ring resonator decides the frequency selection. Hence, keeping the perimeter of the structure same, we vary the resonator dimensions (length and breadth) and investigate and observe the changes, if any, in the output spectrum of all the structures. Simulation has been done through FDTD (Finite Difference Time Domain) method.

P39

SPIN- POLARIZED STRUCTURAL ELECTRONIC AND MAGNETIC PROPERTIES OF 3d (Cr) DOPED SrS

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ABSTRACT

The objective of this study is to investigate the electronic structure and magnetic properties of the dilute magnetic semiconductors alloys SrS doped with chromium impurity. The calculated were performed by using thefull potential linearized augmented plane wave method FP-LAPW within the generalized gradient approximation (GGA) for the electronic exchange and correlation.The lattice constant of Sr_{1-x} Cr_xS decreases with increasing concentration (x) of the Cr atom .we have found that the Sr_{1-x} Cr_xS at all concentration are half metallic ferromagnets with total magnetic moments of 4 μβ per Cr atom.Finally, our predictions require an experimental confirmation in the future.

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P40

THE STRUCTURAL, ELECTRONIC AND THERMODYNAMICAL PROPERTIES OF THE SmX (X = P, Sb, Bi) COMPOUNDS

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ABSTRACT

A detailed theoretical study of structural, electronic and thermodynamical properties of SmX (X = P, Sb, Bi) compounds is presented by performing ab-initio calculations based on density-functional theory Using the package WIEN2K. For describing the interaction between electrons and ions,the full potential linearized augmented plane wave(FP-LAPW) method is used. The generalized-gradient approximation (GGA) is chosen for the exchange–correlation functional . The calculated structural parameters, such as the lattice constant with and without spin-polarization (SP), bulk modulus, the electronic band structures and the related total density of states with SP are presented. For B1 structure, the calculated values of lattice constants are compared with the available experimental and other theoretical data and bulk modulus values are compared with available other theoretical results. In order to gain further information, we have determined the temperature effects on the heat capacities Cv ,debye temperature and thermal expansion coefficient using the nonequilibrum Gibbs function for B1 structure of these three compounds.

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P41

SOLID-LIQUID EXTRACTION OF ORGANIC POLLUTANTS BY MAGNETIC NANOPARTICLES

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ABSTRACT

The objective of this work is to synthesize magnetic particles of raw illite, soda illite, magnetic raw illite and magnetic soda illite from an optimized protocol. the particles are characterized by zetametry, RX, ATG/ATD and FTR. Then their adsorption capacity was evaluated using methylene blue as the adsorbate model. A solid mass equal to 20 mg/10 ml solution, a contact time of 60 min and a neutral pH were found as optimal conditions for the solid-liquid extraction process of methylene blue cations.Under these conditions, crude illite had a maximum fixation capacity of 100.06 mg/g. The results of the kinetic study show that the system follows a pseudo-first order model and a Langmuir adsorption isotherm. The work also includes a study of the separation kinetics of particles synthesized by the application of a magnetic field.

Keywords

Magnetic Illite, Magnetic Illite, Magnetic Illite, Magnetic Illite, Magnetic Illite, Magnetic Separation, Methylene Blue.

P42

FIRST PRINCIPLES STUDY OF OPTOELECTRONIC PROPERTIES IN HALIDE PEROVSKITES $KGeX_3$ (X=Cl and Br), FOR SOLAR CELL APPLICATIONS

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ABSTRACT

We performed a structural and electronic properties of $KGeX_3$ (X= Cl and Br). a theoretical study was carried using the full-potential linearized augmented plane wave method (FP-LAPW) calculations based on the density functional theory (DFT).The exchange correlation potential is treated by using the generalized gradient approximation (GGA-PBE) implemented in the Wien2k package[1] .Lattice parameter (a_0), compressibility modulus (B) and its derivative (B') are determined after the adjustment of total energy (E) obtained from Murnaghan[2] state equation. Cubic halide perovskites $KGeCl_3$ and $KGeBr_3$ shows direct character of theirs band gap in the R-R direction with the values 1.27 and 0.79 eV respectively. The optical properties of these compounds such as the real and imaginary parts of the dielectric function, refractive index, reflectivity and the absorption coefficient are also calculated. The direct band gap and the high absorption of these compounds in the visible and ultraviolet energy range allow these halide perovskites to be a promising nontoxic material for solar cells and laser beam application[3-5].

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P43

MICROSTRUCTURE AND MAGNETIC PROPERTIES OF $Ni_{75}Fe_{25}$ EVAPORATED THIN FILMS: EFFECTS OF SUBSTRATE AND THICKNESS

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ABSTRACT

Permalloy (Py) thin films were evaporated from a nanocrystalline $Ni_{75}Fe_{25}$ powder onto glass and Al_2O_3 substrates [1]. The thickness of these films varies from 16 nm to 250 nm. The as deposited films were characterized by Grazing incidence X-ray diffraction (GIXRD), Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM) and vibrating sample magnetometry (VSM). From GIXRD spectra, we have shown that the films seem to be amorphous for the low thicknesses. However, for the thicker films, a polycrystalline fcc structure is present. For the intermediate thicknesses, the nature of substrate determines the texture of the films. The SEM micrographs indicate that the nature of substrate influences on the morphology and grains size of Py films. From AFM observations, the nanocrystalline nature of the grains is evidenced. Hysteresis loops reveals the ferromagnetic character of Py films. We have shown that the values of coercive field, Hc, generally, decrease with increasing thickness. Moreover, the Hc values are higher for films deposited onto Al_2O_3 substrates than those on glass one. The nature of substrate and thickness seems to influence the magnetic properties of Py films. A correlation between these physical properties will be established and discussed.

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Keywords

$Ni_{75}Fe_{25}$ films, magnetic thin films, thickness, substrate, X-ray diffraction, SEM, AFM, magnetic measurements.

P44

MORPHOLOGICAL AND STRUCTURAL CHARACTERIZATION OF THE Mn-Bi SYSTEM IN NON-AQUEOUS ELECTROLYTE

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ABSTRACT

The present work focuses on the study of the electrochemical kinetics involved in the electrodeposition of the MnBi system in a deep eutectic solvent. This system is known as a hard magnetic material with a large uniaxial anisotropy in its equiatomic phase. A preliminary study of each of the two element has shown that the electrodeposition of Bi is identical to that observed in aqueous electrolyte [1-2] while the electrodeposition of Mn alone was not possible. After adding some complexing agent in the non aqueous electrolyte, the simultaneous electrodeposition of the two elements was made possible in a defined range of potential. The influence of the applied potential on the morphology of the film has been highlighted, it was observed that the deposits have a granular appearance and are more compact when we apply a more cathodic potential. Structural analysis by X-ray diffraction has shown the presence of the characteristic peaks of bismuth and manganese but no peaks characteristics of the MnBi phase was observed. This result is predictable, because the intermetallic phases of MnBi system cannot be formed at room temperature [3]. Annealing treatments under vacuum are therefore necessary to cause the inter-diffusion of the two elements [4].

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P45

FIRST-PRINCIPLES PREDICTION OF STRUCTURAL, MECHANICAL, ELECTRONIC AND MAGNETIC PROPERTIES OF $CuFeX_2$ (X = Se. S)

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ABSTRACT

Several types of ternary and quaternary semiconductors can be proposed as thin films [1]. Among these type of semiconductors, chalcopyrite which are the most promising for the manufacture of thin-film solar cells [2.3]. Of particular interest is the chalcopyrite because of their uses in the different physical domains, photovoltaic [4] chemical and technological domains [5.6]. In this work, we have presented a study on the structural, mechanical, electronic and magnetic properties of $CuFeX_2$ (X = Se. S).The calculations were performed by Ab initio method called FP-LMTO (The full-potential linear muffin-tin orbital) which is based on the formalism of the theory of density functional theory (DFT), using the approximation LDA (approximation of the local density), GGA (generalized gradient approximation) and GGA + U. This allowed us to determine the lattice parameter a_0 , bulk modulus B_0 and its derivative B ', the structure of power and the density of states band, the charge density, the elastic constant. Young's modulus, Poisson's ratio and shear index of refraction. We found that our results are in good agreement with the experimental and other work.

Keywords
chalcopyrite, DFT, Ab-initio, FP-LMTO.

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P46

MAGNETIC OXIDES OF TRANSITION METALS IN THE SYNTHESIS OF NANOSTRUCTURED CATALYSTS

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ABSTRACT

Magnetic oxides of transition metals used to develop materials with catalytic properties usually have magnetic properties. The fact that there is no magnetic remanence in the absence of external magnetic field prevents the formation of aggregates in the reaction medium and thus provides an optimal dispersion of the catalyst. In recent years, numerous articles describe methods of efficient syntheses of magnetic nanoparticles, often of controlled size and morphology. Substantial progress in controlling the size and shape of magnetic nanoparticles has been made by developing methods such as co-precipitation, thermal decomposition and / or reduction, micelle synthesis and hydrothermal synthesis. [1, 2]. Magnetic nanostructures can be used as building blocks for the fabrication of various functional systems, and their application in catalysis and biotechnology [2]. Our work consists of synthesized magnetic nanostructure catalysts by the sol-gel process and studied their behavior. The study methods of its characteristics are multiple: Zeta meter, FTIR, MET, VSM and DRX.

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P47

STRUCTURAL DISTORTION, FERROELECTRICITY AND FERROMAGNETISM IN $PbTiO_{3-\sigma}$

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ABSTRACT

The renewed interest in PTO is due to its potential application as a multiferroic material where a simultaneous ferrolectricity and ferromagnetism can be induced along with a coupling between them. The industrial demand for device functionality is a functional single phase multiferroic material at room temperature with a strong coupling between their ferroelectric and ferromagnetic (FM) order parameters such that they can be easily manipulated either by electric or magnetic field[1]. The tetragonality of $PbTiO_3$ is a signature of enhanced ferroelectric properties and is measured by the c/a ratio which in pure $PbTiO_3$ is ~1.06 at room temperature. And is considerably higher than other perovskite titanates. The ratio decreases with increasing temperature and finally at ~490^0C the tetragonal phase changes to a cubic phase[2]. Synthesis of single phase $PbTiO_{3-\sigma}$ with oxygen deficiency prepared for the first time with PbO and Ti_3O_5 oxides is a challenge which we used solid state reaction method to have a magnetic property for this material.

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P48

STUDY AB INITIO OF HYDROSTATIC TEMPERATURE EFFECT ON A CRYSTALLINE COMPOUND: Sr2YTaO6

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ABSTRACT

By means of Atoms in Molecules (AIM) tools implemented in the abinit code, we attempt to explore local properties of some simple and double perovskite compounds. In our investigation we use algorithms involving a numerical charge density values on a grid. The main standpoint of our focus is decomposing electronic densities and that in order to get partition of the unit the cell in a local volume (v_Ω) and atomic contributions like atomic charge (Q_Ω). This notion of atomic partition allows us to explore the bonding behavior of our compounds by useful and sophisticated methods. We pay attention to the metallization and others phenomena resulting from pressure induced phase transition. Many qualitative ideas about the chemical bond change along these transitions can be quantified from this study.

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P49

MAGNETIC, OPTOELECTRONIC AND THERMOELECTRIC PROPERTIES OF HALF-METALLIC $BaRuO_3$ USING GGA+*U*

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ABSTRACT

We have studied the structural, electronic, magnetic, thermoelectric and optical properties of the half-metal $BaRuO_3$ using the accurate full-potential linearized augmented plane wave (FP-LAPW) method based on the density functional theory (DFT). The generalized gradient approximation (GGA) was used to treat the exchange and correlation potential. The GGA+*U* approximation was also used to enhance the description of the electronic structure after calculating theoretically the Coulomb repulsion (U = 7 eV). The ferromagnetic phase of $BaRuO_3$ is more stable. This result is in accordance with experimental and theoretical calculations. The calculated magnetic moments in $BaRuO_3$ were found to arise especially from the Ru-*4d* state electrons. We have obtained the semiconductor gap (0.9 eV) in spin-up while in spin down, the metal character was dominant, and therefore $BaRuO_3$ has a half-metallic behaviour. The thermoelectric efficiency was 0.12 at room temperature. Here we have considered only the electronic thermal conductivity, we haven't included the lattice thermal conductivity. The relaxation time was assumed constant. The GGA+*U* approximation was also used to analyze the optical properties by determining the complex dielectric function from which are derived the other parameters.

P50

A-B INITIO STUDY OF STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF Ge_n (n=1-19) CLUSTERS DOPED TRANSITION METAL ATOMS USING DFT

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ABSTRACT

In this work we investigate the structural, electronic and magnetic properties of pure germanium clusters as well as the effect of substituting one germanium atom by a chosen transition metal one. By using density functional theory [1] implemented in SIESTA code [2] we study the relation between the electronic, the magnetic properties, the size and the shape of the clusters. We find that the binding energy increases by increasing the clusters size which means that the system continues to gain energy during the growth process. For fixed cluster size, the binding energy depends on the size and the species of doping metal atom. We also find that the HOMO-LUMO gap basically decreases by increasing the size of the clusters. For a given cluster the substituting of one germanium atom by a transition one leads to decrease the HOMO-LUMO gap. Analysing the ionisation potential and the electronic affinity of different clusters, we observe that they decrease and increase, respectively, by increasing the clusters size. Through the magnetic properties of the clusters, analysed by the calculation of the total spin magnetic moment and the total (DOS) and partial (PDOS) densities of states, depend on the shape, the size, the nature and the position of the doping metal transition atom. The chemical hardness shows that the clusters with large size are chemically less stables and more reactive. In addition, the inclusion of platinum atom leads to reduce this stability.

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P51

A COMPARATIVE STUDY OF LATTICE DYNAMICS OF HETEROBILAYER $MoSe_2$ / WSe_2 AND ITS ISOLATED $MoSe_2$ AND WSe_2 MONOLAYERS

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ABSTRACT

2D materials such as graphene, hexagonal boron nitride (h-BN), and transition metal dichalcogenides (MoS_2, WSe_2, etc.) have a very high potential in the fields of energy (electro-catalysis, batteries, photovoltaic), electronics, and optoelectronics. Beyond 2D materials considered individually, composite systems stacks of different layers, called van der Waals heterostructures are particularly attractive: They allow not only to modulate the properties of the materials, but also to further improve their performance. Lattice Dynamics being the basis for a large number of macroscopic properties such as heat capacity, thermal conductivity, and (phonon-limited) electric conductivity is of critical importance for applications in high power conditions where heat dissipation is of pivotal importance.In order to address this issue, we report the phonon dispersion of $MoSe_2$/WSe_2 heterobilayer obtained by a nanostructured combination of isolated $MoSe_2$ and WSe_2 monolayers.The calculations were carried out using density functional theory (DFT) [1,2] taking into account the effect of spin-orbit coupling. The phonon characteristics were calculated within density functional perturbation theory (DFPT)[3]. We found the bandgap of this vertical heterostructure to be smaller than the bandgaps of the subunits while its spin-orbit splitting is intermediate between those of the isolated layers. We also found the existence of three types of phonons, i.e., $MoSe_2$ -like phonons, WSe_2 -like phonons, and hybrid -like phonons. The hybrid phonons originated from the vibrations between the isolated monolayers.

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P52

FIRST-PRINCIPLES STUDY OF ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF DILUTED MAGNETIC SEMICONDUCTOR $Cd_{1-x}Cr_xSe$.

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ABSTRACT

We employ the full-potential linearized augmented plane wave plus local orbital (FP-L/APW + lo) method based on spin-polarized density functional theory (DFT) in order to investigate the structural, electronic and magnetic properties of ordered dilute ferromagnetic semiconductor $Cd_{1-x}Cr_xSe$ (x = 0.25) in the zinc blende (B3) phase. For the exchange-correlation functional, the generalized gradient approximation GGA has been used. Results of calculated electronic band structures and density of states of this dilute magnetic semiconductor are discussed in terms of the contribution of Cr $3d^5$ $4s^1$, Cd $4d^{10}$ $5s^2$ and Se $4s^2$ $4p^4$ partial density of states. Band structure and density of states studies show half-metallic ferromagnetic nature for $Cd_{1-x}Cr_xSe$. Calculations of the s–d exchange constant $N_{0\alpha}$ and p–d exchange constant $N_{0\beta}$ clearly indicate the magnetic nature of this compound. From the calculated total magnetic moments we observe that p–d hybridization reduces the local magnetic moment of Cr from its free space charge value and produces small local magnetic moments on the nonmagnetic Cd and Se sites. The robustness of half-metallicity of $Cd_{1-x}Cr_xSe$ as a function of lattice constant is also discussed.

Key words: Half-metals; Diluted magnetic semiconductors, magnetic and structural properties, DFT

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P53

MAGNETIC, ELECTRONIC AND STRUCTURAL PROPERTIES OF TRANSITION METAL CARBIDES

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ABSTRACT

First-principles calculations are employed to determine the magnetic, electronic and structural properties of transition metal carbides using the the Projector Augmented Wave (PAW) method [1] as implemented in the CP-PAW code and using the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof [2]. density of states, bulk modulus, magnetic moment and ground state properties are determined and compared with available experimental results.

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P54

SPIN WAVES DIFFUSION BY F/AF INTERFACE

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ABSTRACT

This work describes coherent magnons transport in F/AF systems, we develop an analytical and numerical formalism to study the coherent scattering and magnons transport properties via interfaces between ferromagnetic and anti-ferromagnetic thin films. In particular, we study the influence between two ultrathin films composed of five ordered layers. The coherent transmission via the disorder domain, for spin waves incident from the bulk waveguide, is determined with the use of the matching method. Only the nearest neighbors exchange interactions are considered between the spins in the studied model. The effects of varying the local magnetic exchange interaction on the interface zone are calculated and analyzed for three different cases.

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P55

DENSITY FUNCTIONAL STUDY OF CHALCOPYRITE $CuGaSe_2$

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ABSTRACT

A first-principle theoretical study of the structural and electronic properties of CuSe, GaSe and their chalcopyrite system, has been performed using the full-potential linear augmented plane wave (FP-LAPW) method. The generalized gradient approximation (PBE-GGA) was used for the exchange and correlation energy density functional. In particular, the lattice constant, bulk modulus and band gap energies of CuSe and GaSe compounds and their chalcopyrite system CuGaSe2 are calculated and discussed. We found, that the parent materials present half-metallic behavior for GaSe in zinc blende phase and CuSe gives the Fermi level situated in valence band, so the metallic behavior. But the chalcopyrite system offers a direct large band gap at Γ (1.19 eV).

Keywords: $CuGaSe_2$ chalcopyrite, Wien2K, Structural property, Electronic properties.

P56

MÖSSBAUER SPECTROSCOPY OF $Fe_{60}Al_{40}$ NANOSTRUCTURED POWDERS

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ABSTRACT

We have studied the effect of milling time on the hyperfine properties of $Fe_{60}Al_{40}$ powders prepared by mechanical alloying. A series of samples was prepared in a friction mode for different milling times ranging from 6 h to 72 h. The analysis of Mössbauer spectra was performed with win-normos software. the results of the analysis show the existence of different environments with increasing milling time. Indeed, for milling time of 6 h and 12 h, the Fe(Al) solid solution starts to form and increases in intensity. After 12 h of milling, we noticed a total formation of Fe(Al) solid solution showing the presence of different FeAl phases. For a milling time of 72 h, the adjustment of Mössbauer spectrum shows the existence of only a sextet with a mean hyperfine field of 24 T indicating the formation of binary $Fe_{60}Al_{40}$ alloy.

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P57

GGA+U STUDY OF STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF PrCrO3 CUBIC PEROVSKITE

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ABSTRACT

First principles calculations based on density functional theory have been employed to study the structural, electronic and magnetic properties of PrFeO3 perovskite.The calculations were performed by full potential linearized augmented plane wave method with generalized gradient (GGA) and GGA+U approximations for the exchange and correlation functionals. The electronic properties show that PrCrO3 exhibits a complete half-metallic character for both approximations GGA and GGA+U with integer magnetic moment, while the value of eV is the most appropriate for PrCrO3.

P58

NANOCOMPOSITE: A COMPARISON BETWEEN GRAPHENE AND CARBON NANOTUBE AND THEIR BEHAVIOR

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ABSTRACT

Nanotechnology is the study of structures at the scale of the nanometre. The composite material is becoming commonly used nowadays, research in the field of composites and nanocomposites are booming. Our perception of materials is to be challenged by recent studies in many fields of engineering. The study of nanomaterials is in full swing and evolving, full of promise, towards a revolution of our perception of materials in many fields of engineering. In this work reviews the processing techniques for developing nanocomposites. We limit the discussion to 1D and 2D fillers of nanocomposites as it has been reported that 2D fillers provide a higher degree of reinforcement than spherical shaped (3D) fillers; we give a comparison between the carbon nanotubes and the graphene fillers in polymeric matrices and conventional composite materials, and their electrical and thermal and mechanical properties.

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P59

FIRST PRINCIPAL CALCULATIONS OF STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF NICKEL AND COBALT DOPED PHOSPHORUS CLUSTERS MPn FOR M=Ni; Co; (n = 1 – 24).

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ABSTRACT

In this work, we report ab initio calculations of equilibrium geometries, electronic and magnetic properties of Mp_n for M=Ni; Co (n = 1−24) clusters by using the first principals density functional theory (DFT) approach within the generalized gradient approximation (GGA) implemented in SIESTA simulation package. The relative stabilities have been studied in terms of the binding energies, the second-order difference of energies, the HOMO-LUMO gaps, the verticals ionization potentials and electronic affinities and the chemical hardness for all pure and doped structures. The obtained results show that the binding energies generally increase with the increasing of cluster size which indicating that the clusters continue to gain energy during the growth process. The evolution of the electronic structure can also be probed by calculating the characteristics of the energy gap between high occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The theoretical HOMO–LUMO gaps of the most stables MP_n clusters are generally decreases as the cluster size increases. This indicates that the MP_n clusters with large size seem to be approaching the gap closure characteristic of a metallic state which is enhanced by the doping M atom and consequently the highest chemical reactivity. The MP_8 which have the largest HOMO-LUMO gap cluster has high stabilities when compared to their neighboring clusters. The magnetic properties of MP_n clusters are discussed according to the value of the total magnetic moment calculated for the lowest energies structure. The magnetic moment of MP_n depend on the structure and symmetry of given clusters and on the position of M atom and the number of his neighboring P atoms. We have also explored the vertical electron affinity (VEA) and the vertical ionization potential (VIP) of MP_n clusters. We find that there are odd-even alternation in both VEA and VIP as a function of size of MP_n clusters. This means that some MP_n clusters have specific properties and they are more stables than the neighboring clusters.

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P60

FIRST-PRINCIPLES STUDY OF HALF-METALLICITY IN ALKALI-METAL CHALCOGENIDES COMPOUNDS: NaX (X = S, Se, Te)

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ABSTRACT

The discovery of magnetism in a wide variety of compounds that do not contain transition metal or rare earth ions have led to increased research interest [1, 2] due to their possible applications in spintronic. In this work, the structural, electronic and magnetic properties of NaX (X = S, Se, Te) alkali-metal chalcogenides binary compounds have been investigated by the first-principles full-potential linearized augmented plane-wave method based on density functional theory in different crystalline phases: NaCl, CsCl, ZB, NiAs, WZ and *Pnma*. We found that the most stable phase for the NaX binary compounds is the non-magnetic *Pnma* phase. Our calculation has been carried out within the Perdew-Burke-Ernzerhof (PBE) under generalized gradient approximation (GGA) and the modified Becke-Johnson (mBJ-GGA) for the exchange-correlation energy and potential. As far as we know, it is the first time to research the detailed electronic structures, and magnetic properties of these compounds. The calculated lattice parameters, bulk moduli, their first-pressure derivatives and internal parameters are in good agreement with the other theoretical data. The electronic band structure and density of states show that half-metallic and magnetic character arises, which can be attributed to the presence of spin polarized *p* orbitals in the group VI elements. The NaS, NaSe, and NaTe binary compounds show half-metallic character in ZB and WZ phases, with an integer magnetic moment of 1 μ_B per formula unit and half-metallic gaps.

Keywords: Density functional theory; Half-metals; Ferromagnetism; Alkali metals; Chalcogenides.

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P61

MAGNONIC SCATTERING VIA NANOJUNCTIONS IN BCC WAVEGUIDES

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ABSTRACT

A calculation of the coherent and ballistic magnonic transport via thin nanojunction between bcc lattices is presented. The model system A/B/A consists of a finite number of bcc atomic layers of an element B integrated between two bcc semi-infinite ferromagnetically ordered crystals A. Transmission and reflection scattering cross sections are determined from elements of a Landauer type scattering matrix. The theoretical calculations are carried out using the matching procedure and Landauer-Buttiker formalism. The calculated properties are presented for arbitrary incidence angles of the magnons on the boundary, for all accessible frequencies in the propagating bands, and for the interatomic magnetic exchange of the A and B subsystems, and their spin intensity, with no externally applied magnetic field. Numerical results show characteristic interference effects between the incident spin waves and the localized spin states of the nanojunction.

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P62

AB-INITIO CALCULATIONS OF THE ELASTIC, MAGNETIC AND ELECTRONIC PROPERTIES FOR THE MPt [M= Fe, Ni, Cr, Cu, Co] THIN FILMS.

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ABSTRACT

Materials with high perpendicular magnetic anisotropy (PMA) have received considerable attention for ultra-high-density magnetic recording media fabrications. We study here the elastic, magnetic and electronic properties of the (001) orientation in the L_{10} phase of MPt [M= Fe, Ni, Mn, Cu, Co] thin films with 9 layers. The calculations were performed in the framework of the DFT as implemented in VASP code. The ion-electron interaction was described by PAW pseudopotentials. For the exchange-correlation interaction, the Perdew, Burke and Ernzerhof (PBE) GGA approximation was used.

From the calculated surface energies, we obtained the stability order of MPt thin films following the order: MnPt< FePt < CoPt <NiPt< CuPt. The elastic constants were calculated for the two-dimension (2D) MPt structures. Young's modulus and Poisson's ratio have been also determined. We find that these 2D-structures are mechanically stable. The total magnetic moments change strongly in the following order M(MnPt)> M(FePt)> M(CoPt)> M(NiPt). The density of states diagrams have been also calculated and analysed.

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P63

MAGNETIC AND ELECTRONIC PROPERTIES OF CFC ORDERED DOUBLE PEROVSKITE HALF-METALLIC BEHAVIOR, FERROMAGNETIC COUPLING PREDICTED BY FIRST-PRINCIPLE CALCULATIONS

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ABSTRACT

In this paper, the magnetic, electronic and structural properties of Sr_2BOsO_6 where B= Ca and Sc ordered double perovskite based osmium has been calculated with the full potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT) as implemented in the Wien2k package, using generalized gradient approximation (GGA) and GGA plus trans-blaha-modified Becke–Johnson (TB-mBJ) as the exchange correlation. According to the structural results such as the lattice parameters is in good agreement with the previous experimental data, where the cell parameter is 8.02 Å and 7.92 Å respectively for Sr_2CaOsO_6 and Sr_2ScOsO_6. Spin-polarized electronic band structure and density of states present 100% of spin polarization at Fermi level for these compounds, resulting in half-metallic behavior grand state with the ferromagnetic coupling of B and Os spins with B= Ca and Sc respectively for Sr_2CaOsO_6 and Sr_2ScOsO_6; the total magnetic moment amounts to μ_T=2.000μ_B and 3.000 μ_B respectively for Sr_2CaOsO_6 and Sr_2ScOsO_6, whereas the most contribution is by the osmium atom in both compound. Based on the electronics results, the Sr_2CaOsO_6 and Sr_2ScOsO_6 double perovskite compounds have a direct band gap in (Γ-Γ) direction with a value of 2.062 eV and 2.453eV respectively, making these materials competent candidates for optical and spintronic applications, on other hand, this study can light the way for more investigation of this popular complex oxide perovskite material for various chemical and physical applications.

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P64

SURFACE MAGNETIC EXCITATION WITHIN INFLUENCE DZYALOSHINSKII–MORIYA TERM IN THE WEAKLY NON-COLLINEAR CONFIGURATION APPLICATION TO MF_3 STRUCTURE (M= Fe, Cr).

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ABSTRACT

In this study, we have theoretically investigated the influence of the anisotropy field and the Dzyaloshinskii-Moriya (D-M) type coupling on bulk and surface spin excitations. Two applications of the formalism developed here have been done on the trifluorides MF_3 (M=Fe, Cr) structures which provides a good illustration of the presence of magnetic frustration due to competing interactions and the existence of non-collinear structures. In the first part the bulk and surface spin dynamics are analyzed under the influence of anisotropy field whereas in the second step the antisymmetric interaction (D-M) is considered thus enabling a detailed analysis on the influence of the Dzyaloshinskii-Moriya (D-M) term on the propagating and evanescent precessional fields occurring in the neighborhood of the bulk-surface region. The bulk-surface spin dynamics are studied using theoretical formalism based on the symmetry properties obtained from the semi-infinite system by examining the matching equations for evanescent and propagating solutions deduced from the bulk secular equation, satisfying surface boundary conditions. The calculations have been carried out considering the competing inter-sublattices nearest and intra-sublattices next nearest neighbors exchange interactions occurring in the bulk and surface. It was found that the spin wave dispersion associated with the bulk as well as with the surface are strongly dependent on the values of ratio of bulk-surface parameter (J_S/J_{AB}) and the canting angle Θ. An energy gap which illustrates a new magnetic ground state for surface spin quantum configuration is evidenced. In addition, it was observed that this energy gap increases as the non-collinearity increases.

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P65

AB-INITIO STUDY OF OPTOELECTRONIC, ELASTIC AND MAGNETIC PROPERTIES OF CUBIC $GdCrO_3$ PEROVSKITE

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ABSTRACT

Theoretical investigation on electronic structural, mechanical, magnetic and optical properties of cubic $GdCrO_3$ perovskite oxide has been accomplished within density functional theory (DFT). The exchange correlation potentials is treated by the generalized gradient approximation (GGA), GGA+U and GGA plus Trans-Blaha-modified Becke–Johnson (TB-mBJ) which have been used to correct the potential. The calculated lattice parameters agree well with the experimental measurements. The elastic constants results and their related parameters (Young modulus, shear modulus, Poisson ratio, Zener anisotropy) show clearly that the $GdCrO_3$ perovskite is a ductile, stiff and anisotropic material. Density of States and band structure results reveal a metallic ferromagnetic characteris of $GdCrO_3$ using GGA method whereas half-metallic ferromagnetic ground state is obtained when using GGA+U and TB-mBJ approximations. The integer value of the total magnetic moment of 10,00 μB confirms the half metallicity for our compound. Furthermore, we have computed the dielectric function, optical reflectivity and absorption coefficient which are investigated for the first time. These results make $GdCrO_3$ a promising candidate for optoelectronic and spintronic applications.

P66

AB-INITIO CALCULATION OF STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF LAYERD TRANSITON METAL DICHALCOGENIDE (LTMDs)

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ABSTRACT

We present the structural and electronic properties of layered transition metal dichalcogénide (LTMDs) $MoSe_2$ and Wse_2 monolayers and Wse_2 / $MoSe_2$ heterobilayer. The heterostructure resulting from this layer-by-layer assembly allows to construct devices that basically preserve the properties of their subunits without almost any degradation and give rise to novel properties to be applied in nanoelectronics. Our ab-initio calculations are carried out by using Density Functional Theory (DFT) [1,2] and Many-body Perturbation Theory (MBPT) based on the Green Function Method (GW approximation) [3,4]. The band structure calculations show the isolated layers to be direct gap semiconductor at the K point of the hexagonal Brillouin zone in the visible range, while the heterobilayer is found to exhibit type -II band alignment (GW level) with an indirect gap being in agreement with experimental evidences. Furthermore, the effect of spin orbit coupling on the electronic band structure are tested. It is found that the inclusion of this relativistic effect splits the top of the valence band and the bottom of the conduction band thus decreasing the band gap width. Our results provide key ingredients to design van der Waals materials with tailored characteristics.

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P67

AB-INITIO STUDY OF HALF-METALLIC FERROMAGNETISM IN GeNaX (X = Ca, Sr, Ba) TERNARY HALF-HEUSLER ALLOYS

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ABSTRACT

The half-Heusler XYZ and the full-Heusler X2YZ compounds without transition metals mainly referred to as d^0 half-metallic ferromagnets (HMF) still a field of active research [1, 2]. They have attracted great interest due to their possible applications in spintronics. In this work, the electronic structures and magnetic properties of GeNaX (X = Ca, Sr, Ba) ternary Heusler alloys have been investigated by the first-principles approach based on density functional theory (DFT) and the full-potential linearized augmented plane-wave (FP-LAPW) method in different crystalline phases: α, β and γ. We found that the most stable phase for the GeNaX (X = Ca, Sr, Ba) ternary Heusler alloys is the α phase. Our calculation has been carried out within the Perdew-Burke-Ernzerhof (PBE) under generalized gradient approximation (GGA) and the modified Becke-Johnson (mBJ-GGA) for the exchange-correlation energy and potential. As far as we know, it is the first time to research the detailed electronic structures, magnetic, mechanical and thermo dynamical properties of GeNaX compounds. GeNaCa, GeNaSr and GeNaBa ternary Heusler alloys were found indirect band-gap compounds, and the calculated half-metallic band gaps by using GGA(mBj-GGA) are respectively 0.26(0.59), 0.39(0.66) and 0.08(0.33) eV. In all the cases ferromagnetic phase is energetically favored with respect to the paramagnetic one in the α and β structures. We also consider the effect of pressure on the half-metallicity of these compounds and we find that these compounds in the α phase maintain their half-metallicity under volume compression. It is shown that our calculated structural and magnetic properties are in good agreement with the available theoretical results. We have also calculated the density of states, elastic moduli and the phonon dispersion relations of the GeNaX (X = Ca, Sr, Ba) ternary Heusler alloys in the α phase. Moreover, we determine phonon dispersions, phonon density of states, thermodynamic properties in these compounds. These properties cause GeNaX (X = Ca, Sr, Ba) ternary Heusler alloys to be appropriate choices to create useful devices in spintronics.

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P68

VACANCY EFFECT ON THE MANGANESE MAGNETIC MOMENT IN FCC FE-MN ALLOY: DFT STUDY

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ABSTRACT

Calculations based on the pseudo-potential density functional theory (DFT) were performed to study the structural and magnetic properties of fcc Fe with one vacancy and 3 at.% of Mn. Our results reveal that, energetically, manganese atom and vacancy prefer to occupy the most distant sites from each other and reveal also that manganese concentration and vacancy location with respect to Mn affect the Fe-Mn magnetic interaction. With presence of one vacancy in Fe-Mn alloy, the local magnetic moment of manganese changes sharply.

Keywords: FeMn alloy, magnetism, ab initio calculations.

P69

ELECTRONIC, MAGNETIC AND THERMOELECTRIC PROPERTIES OF OXIDE NITRIDE PEROVSKITE

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ABSTRACT

Oxide nitride perovskites, where the oxide ions are partially replaced by nitride ions, constitute a large class of materials with a variety of interesting properties and important technological utility. Recent studies on some nitride oxide perovskites have revealed colossal magnetoresistance ,paramagnetism, ferrimagnetism, and spin glass behavior. In the $RTiNO_2$ class, $NdTiNO_2$ is reported to possess Pnma space group symmetry, which is quite common for perovskites. The measured effective magnetic moment for $NdTiNO_2$ is 3.47 μB. A density functional theory (DFT) employing generalized gradient approximation (GGA) and modified Becke Johnson (TB-mBJ) potential have been used to study the electronic and magnetic properties of $NdTiNO_2$. Based on the electronic results, the temperature dependence of the thermoelectric properties of $NdTiNO_2$, were investigated in temperature range from 100K to 1200K.

P70

INFLUENCE OF THE SUBSTRATE AND THICKNESS ON MORPHOLOGICAL AND MAGNETIC PROPERTIES OF PERMALLOY THIN FILMS

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ABSTRACT

We report the effect of the substrate and the thickness on the microstructural and magnetic properties of permalloy thin films elaborated by physical vapor deposition. The films thicknesses range from 16 to 90 nm, the glass, silicon and quartz where used as a substrates. From the morphological observations of the films, the Py/ glass and Py/ Si presents a smooth surface while le Py films deposited on quartz exhibits a very rough surface. The magnetic measurements show that both for Py/glass and Py/Si series, the coercivity is less than 7 Oe. Concerning the Py films deposited on the quartz substrate, the sample having 25 nm in thick, present the higher coercivity equal to 80Oe. It is also observed that these samples need high magnetic fields to saturate.

Keywords: Permalloy film, morphology, magnetic measurements.

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P71

FIRST-PRINCIPLES INVESTIGATIONS OF MAGNETIC PROPERTIES OF FE/IR/CO

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ABSTRACT

The aim of our work is to investigate the magnetic properties of Fe/Ir/Co by first principles calculations using full-potential linearized augmented plane-wave (FLAPW) method as implemented in the FLEUR code which it is based on density functional theory. It was found that the magnetic ground state is ferrimagnetic configuration it means ferromagnetic coupling between Co atoms and antiferromagnetic coupling on Fe layer. For the magnetic moment, the Fe moment is 2.83 μ_B and it is 1.84 μ_B for Co atoms. Finally, we show that the interlayer exchange coupling (IEC) between the Fe and Co layers has the oscillatory behavior between FM and AFM coupling and has strong coupling at very low thickness.

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