Ministère de l'Enseignement supérieur et de la Recherche scientifique

Université des Sciences et de la Technologie d'Oran Mohamed-Boudiaf USTOMB

Laboratoire de Physique des Matériaux et des Fluides -USTO-MB

CPMF 2022

Conférence sur la Physique des Matériaux et des Fluides

Du 18 au 19 Décembre 2022

-Les Andalouses-

Oran (Algérie)

Contents

Conference Program

Sunday, December 18, 2022

09h30mn-10h Opening Ceremony

Plenary Session :

Chairman: Pr H.ALLA

01	10h-10h30’	Pr. Hafid Aourag	Université de Tlemcen
02	10h30’-11h	Pr. Zheyu Lieu	College of Petroleum Engineering, China University of Petroleum, Beijing, China.

11h-11h30mn Coffee Break

Chairman : Pr H.Aourag

03	11h30’-12h’	Dr. Thibault Roques-Carmes	LRGP – ENSIC – University of Lorraine, Nancy, France
04	12h-12h30’	Dr. Mohamed Khodja	Head of Research – SONATRACH/IAP Boumerdes, Algeria.
05	12h30’-13h	Pr. Bachir Bouhafs	Physic’s Department, Sidi Bel-Abbes, Algeria.

13h-14h Lunch Break

Oral Session

	EOR-RS Chairman : Dr M. Khodja	NME Chairman : Pr B.Bouhafs	NSN Chairman : Pr N.Adnane	CE Chairman : Dr Khellil
14h-14h20’	Farouk Selmi	Wassila Sekkal	Lounis Belhimer	Fatéma Ammour
14h20’-14h40’	Abdallah Sokhal	Hakima Boublenza	Nadia Houri	Bachir Nail
14h40’-15h	Sabeur Amine	Mohamed Abdelilah Fadla	Siham Djoumi	Ali Reguieg
15h-15h20’	Miloudi Hafida	*Samir Meziani*	Tahir Ghazoul	**RM Chairman : Pr N.Belkaid** Amirouche Bouremani
15h20’-15h40’	Laroussi Kada	*Hadj Moulay Ahmed Mazouz*	Cheikh Imene	
15h40’-16h		Yazid Zakaria Hamri	L. Asma Kawther	

16h-16h30mn **Coffee Break** ***Poster Session***

Chairman : Pr. M. Messad

	FM **Chairman :** **Dr.Y. Laghouati**	**NME** **Chairman :** **Pr. D. Madouri**	**NMM** **Chairman :** **Pr M. Elchikh**	**NMM** **Chairman :** **Pr S.Hiadsi**
16h30'-16h50'	Kouadria Amar	Oussama Bachir Bouiadjira	Aida Benmalek	A.Hireche Baghdad
16h50'-17h10'	Oussama Mebarki	Yazid Zakaria Hamri	M.H.M. Belhachemi	Asma Kadri
17h10'-17h30'	Abderezak Bennia	Nasreddine Bouziane	F.D.Benyahlou	
17h30'-17h50'	Tarek Sriba	Mahdjouba Khatiri		

Monday, December 19, 2022

Plenary Session :Chairman : Pr. M. Abdelouahab

01	**09h30'-10h**	**Pr. Ali Zaoui**	**Lille Polytechnic, France**
02	**10h-10h30'**	**Dr. Wörner Martin**	**Karlsruhe Institute of Technology, Germany**
03	**10h30'-11h'**	**Pr. Alla Hocine**	**Université des Sciences et Technologies USTO-MB**

11h-11h30mn Coffee Break

Chairman : Pr. M. Elchikh

04	**11h30'-12h**	**Pr. Marco Marengo**	**Director of the Advanced Engineering Centre, University of Brighton, UK**
05	**12h-12h30'**	**Pr. Yacine Salhi**	**Université sciences et technologie Bab Ezzouar USTHB**

12h30-13h30 Lunch Break

Oral Session

	EOR-RS Chairman : Dr. A. Deghmoum	**NME Chairman : Dr H.Boublenza**	**PCE Chairman : Pr S.Bendella**	**FM Chairman : Dr. O. Bentata**
13h30-13h50'	*Karima Hammadi*	Loubna Benhabib	Soumia Bendella	Sara Yousfi
13h50-14h10'	*Farouk Selmi*	M.A.Charef	Aicha Djaraba	Samira Bekhadra
14h10-14h30'	Yacine Salhi	Khadraoui Zakaria	Fatiha Ghaleb	
14h30-14h50	Noujoud Meskoud	Azzi Saliha	Khadidja Khodja	
15h10-15h30	Abdellah Sokhal			

15h30-16h00 Coffee Break *Poster Session*

Chairman : Pr. H. Ait Kaci

16h00-16h30 Work Meeting & Closing Ceremony

Liste des plénières :

N°	Noms Prénoms	Titre de la communication
1	**Pr Hafid Aourag**	How New advanced ultra hard materials have reshaped the industries of oil and gaz.
2	**Pr Bachir Bouhafs**	Cu-based Half-Heusleur alloys for spintronic device: ab-initio prediction of new stable phases.
3	**Dr Thibault Roques-Carmes**	Chemical Product Design Methodology applied to Formulated Products and Enhanced Oil recovery EOR
4	**Pr. Zheyu Lieu**	Insights into the role of in-situ emulsification in a surfactant/polymer-light oil system with ultra-low interface tenstion on enhanced oil recovery
5	**Dr. Mohamed Khodja**	Fluides de forage, EOR et Laitiers de ciments.
6	**Pr. Ali Zaoui**	Clays and their role in the protection of environment and human life
7	**Dr. Wörner Martin**	An energy balance model for the maximum spread diame-ter upon droplet impact on surfaces of arbitrary wettability
8	**Hocine Alla**	Design of the chemical EOR by numerical solutions adapted difficult conditions of the reservoir in Algeria
9	**Pr. Marco Marengo**	Simulating vapour nucleation at nanoscale through diffuse interface modeling.
10	**Pr. Yacine Salhi**	Two-phase flow in macro and microchannels

Liste des communications orales :

EOR-RS	Nom	Titre
1	Farouk Selmi	Evaluation of the effect of Polymer Flooding on Increasing Oil Recovery and Reducing Barrel Cost.
2	Abdallah SOKHAL	Rock Type Classification Using,vMachine Learning Algorithms withvPython in Algerian Triassic Sandstone Reservoir
3	Sabeur Amine	Molecular Dynamics simulation of the injection of polymer chains into a nanopore for enhanced oil recovery operations
4	Miloudi Hafida	Microemulsion in EOR
5	Laroussi Kada	pilot design for a test bench pour l'EOR
6	Karima Hammadi	Simulation of injection gas miscible CO 2 and alternative injection of water and gas miscible CO 2 in oil reservoir-case study from Algerian
7	Farouk Selmi	Sensitivity Study of SCAL Parameters on the Performance of WAG Injection Process on Hassi Messaoud Field

8	Yacine Salhi	Numerical simulation of CEOR processes - case studies.
9	Noujoud Meskoud	Performances & uncertainties of the chemical EOR process on Algerian field

NME	**Nom**	**Titre**
1	Wassila Sekkal	Advanced green building material for a promising environmental sustainability
2	Hakima Boublenza	First-principles study of optoelectronic properties of Cu-based chalcogenides
3	Mohamed Abdelilah Fadla	Mixed halide perovskite for solar energy conversion, Alloys and their effect on material stability
4	*Samir Meziani*	Development of selective emitter solar cells with laser doping
5	*Hadj Moulay Ahmed Mazouz*	Electronic structure, Magnetic and dynamical properties of RbS and CsS : ab initio insight
6	Yazid Zakaria Hamri	Simulation of thin film solar cells of CIGS with AMPS-1D software
7	Oussama Bachir Bouiadjira	Organic MA cation A-site doping in CsPbI 3 perovskite by first principle calculations.
8	Yazid Zakaria Hamri	Numerical modeling of ultra thin Cu(In, Ga)Se2 solar cells
9	Nasreddine Bouziane	Defect density influence of the crystalline silicon for the structure ITO/a : Si-H/c-Si/Al in the dark and under illumination
10	Mahdjouba Khatiri	First-principles study of the Heusler superconductors Ni 2 ZrX (X= Ga and Al)
11	Loubna Benhabib	Optimization of the photovoltaic efficiency of a cell based on GaAs
12	M.A.Charef	Les biopiles a compbustible biologiques une application pretinante des energies renouvelable
13	Khadraoui Zakaria	DFT study of the structural, electronic and optical properties of the CoFeRuSn Quaternary Heusler compound.
14	Saliha Azzi	Ab-initio study of the electronic structure of Barium Oxide BaO and the $NaBa_3O_4$ alloy

NSN		
1	Lounis Belhimer	The effet of carbon nanotube on microelectronic
2	Nadia Houri	Porous Carbon as low cost Pt-free counter electrode for dye-sensitised solar cell
3	Siham Djoumi	Tin and Indium promoted Silicon Nanowires growth via plasma assisted vapor liquid solid process
4	Tahir Ghazoul	Nano-reinforced composite structures on elastic foundation: free vibration analysis
5	Chikh Imene	Elaboration and Characterization of a New PVA-CMC/Fe_2 O 3 Semiconductor Composite Biomaterial

6	Asma Kawther Lachachi	Electrical properties and affinity towards hydrogen to the nanoparticuls Cu 0 -loaded SBA-15@ZnO
FM		
1	Kouadria Amar	Performance hydrodynamiques de mélange des fluids non-Newtoniens dans des dispositifs microfluidiques passifs
2	Oussama Mebarki	Numerical study of the motion of a solid particle carried by a gas in a micrometric system
3	Abderezak Bennia	Cooling of electronic components using convective fluids
4	Tarek Sriba	Numerical simulation of the creation and diffusion of a vortex ring in a non-Newtonian fluid.
5	Sarra Youcefi	Numerical simulation of newtonian and non-newtonian fluid flow in a singularity
6	Samira Bekhadra	Numerical simulation of blood flow in the bifurcation of the carotid artery
CE		
1	Ali Reguieg	Experience of the CHUO neonatology service during the COVID 19 pandemic
2	Bachir Nail	Controlling COVID-19 outbreak in Algeria using metaheuristic optimization algorithm.
NMM		
1	Aida BENMALEK	Doping and co-Doping Impact on the Structural, Electronic and Magnetic properties of CeO2 : based on first principle calculation
2	Mohammed Hadj Mortada BELHACHEMI	Homo-lumo, global chemical reactivity descriptors and nonlinear optical properties of 1-benzyl-5-methylindoline-2,3-dione
3	Zohra Douaa BENYAHLOU	Theoretical study of charge transfer, chemical reactivity and nonlinear optics application for a new organic molecule
4	A.HIRECHE BAGHDAD	Theoretical investigations study of structural, mechanical and Optoelectronic Applications of ternary semiconductors YAgTe2 under high pressure.
5	Asma Kadri	Investigation of Various Properties of Anti-perovskite Based Rare Earth AlNSc3.
PCE		
1	Soumia BENDELLA	The influence of ammonia on a discharge dbd of ar
2	Aicha DJERABA	Study of measuring bone mass density by dual x-rays absorptiometry
3	Fatiha Ghaleb	The role of silane reactions kinetics on the density distribution in plasma discharges for silicon deposit
4	Khadidja Khodja	Enhanced hydrogen generation by converting pure methane using DBD
RM		
1	Amirouche BOUREMANI	Mathematical modeling of the thermoluminescence (I-TL) in SrY2O4:Eu3+

Liste des communications poster :

Nom et Prénoms	Session Poster EOR-RS
Hasnia Benmoussa	Green and rapid extraction of essential oil from Algerian Origanum majorana
Fatima Bekkar	Amélioration de la récupération assistée du pétrole par injection de Surfactants-polymères
Hanene Zahaf	Design of the chemical EOR by numerical solution adapted difficult conditions of the reservoir in Algeria.

Nom et Prénoms	Session Poster NME New materials for renewable energies (Photovoltaic, thermoelectricity, energy storage (battery))
Adel Allal	Oxygen-functionalized W2C MXene as anode material for Na-ion battery: A first-principles study
Ouafaa Sadouki	The theoretical prediction of cumg 2 als 4 quaternary chalcogenide
Mama Hamlat	Enhancement of the magneto-electronic properties by GGA and TB-mBJ approaches for KBeO3 perovskite oxide”
Ouafa Hamidane	The investigation on structural, electronic, magnetic and thermodynamic properties of half-metallic materials via first-principles calculations based on density functional theory”
Nezha Benyahia	Comparative study of optoelectronics, mechanical, dynamic properties of GaAs, GaP, and GaAsP Compounds
El Habib Abbes	Investigation of structural, electronic, magnetic and half-metallic properties in ternary Half-Heusler alloy FeVGe : FP-LAPW calculations
Imene Bouhamou	Ab-initio investigation of structural, electronic and elastic properties of Ru2CuGe full-Heusler alloy
Mohamed Lamine Belkhir	ab-initio study on the structural, electronic, magnetic, elastic, dynamical stability of quaternary heusler alloys rhcovsi rhcovge and rhcovsn
Nesrine Hamidane	Ab initio calculations of the fundamental properties of half-metallic materials : Possible Candidates for modern spintronics devices
Asma allouche	“Structural,electronic, optical and thermoelectric properties of halide double perovskite Cs2AgBiX6 (X= F ,Br) : DFT study ”
N. E. A. Doghmane	Approximations choice and adequate conditions for the investigation of ZnO properties”
Bourahla Asma	First Principle calculations of structural, elastic, electronic and magnetic properties of Ag 2 BSm

	full Heusler alloy compounds using GGA and GGA+U: FP-LMTO calculations
Youcef Guermit	Investigation théorique des propriétés structurelles électroniques et thermodynamiques de l'alliage Mn2ScSi.
Nassima Hammou	Relativistic effects on the structural, electronic and dynamic properties of new hypothetical III-V compounds formed by the group III elements and superheavy element of group V
Souheil BELBACHIR	First-principle study of Physical properties of new half-metallic quaternary Heusler alloys: CoZrYP (Y=Mn and Fe).
Lilia Beldi	Ab-initio study of electronic structure and magnetism in the rare-earth-based half-Heusler GdPdBi alloy.
Zohra Choualhi	Etude ab-initio de la structure électronique de l'élément Ag
Belmiloud Nawal	Electronic, elastic and lattice dynamical properties of the half Heusler alloys KMgX (X =P, As)
Nom et Prénoms	Session Poster New materials for renewable energies (Photovoltaic, thermoelectricity, energy storage (battery))
Samira Touat	Ab-initio study of structural, elastic, electronic, and magnetic properties of Mn2FeAl full-Heusler alloy.
Khadidja Fatima Zohra NAIR	Prediction of the structural, mechanical and thermodynamic stability of the half-Heusler NiMnAs alloy.
Hamri Asma	First-principles study of the half-metallic behavior in the full-Heusler Co2MnV alloy.
Hamri Imène	Stability and magnetism in the quaternary Co2CrTixV1-x full-Heusler alloy.
Hamida Heddar	Magnetic properties of GaN/(MnN)n/AlN/((CrN)n, aN/(MnN)n/AlN/((VN)n,GaN/(CrN)n/AlN/((VN)n superlattices (n= 1, 2)
Fadila Belkharroubi	Investigation of Structural, Elastic, Magnetic and Electronic proprieties for Co2LuAs Full-Heusler Alloys
Hocine Kamel	The Structural, Electronic, Optical properties of Oxynitride Perovskite CaTaO2N
Djazia Nasri	Ab initio study of structural, electronic and magnetic properties of V-doped ZnS
M. Lebaad Benhafsa	First-principles calculations of structural, elastic, dynamic, electronic, and magnetic properties of Co2FeSi full-Heusler alloy.
HAMRI Bouabdallah	Theoretical investigation of structural, electronic and magnetic properties of Ti-based full-Heusler alloy.
Kara Ilham	Theoretical study of the structural electronic properties of half-Heusler KInSn alloy
Rahmani Rabea	First principles calculations of structural and optoelectronic properties of XF 3 (X= La, Al)
Fatima Zohra Maroc	Study of the physical characteristics of sodium halides in interaction with X-rays
Hayet Sediki	First principles calculations of electronic and magnetic properties of Perovskite NdGdO 3 : a theoretical study
Djezzar Nor El Houda	Investigating new stable phases for the ternary alloy II-VI of Sr x Ca 1-x O: DFT study
Mebtouche Hanane	First-principles calculations of the structural, electronic, mechanical and thermodynamic properties of MAX Phase Mo n+1 GeC n (n = 1, 2, and 3) compounds
Halles El Ajal	First-principles study of structural, electronic, magnetic properties and elastic anisotropy of Sr 1-x TM x S (TM = Fe, Co)
Mazouz Moulay	Electronic structure, Magnetic and dynamical properties of RbS and CsS : ab initio insight

Nom et Prénoms	**Session Poster** **Fluid Mechanics : Two-phase flows**
Douroum Embarek	Parametric study of the effect of the crossing elongation on the mixing performances of a compact microfluidic system
BENALI AEK	Numerical investigation of the hydrodynamic aspect of a liquid-liquid extraction column at various stirring speeds

Nom et Prénoms	**Session Poster** : PCE Plasma and conductive energy
Halima LOUKIL	Experimental study of the electrical and optical characteristics of plasma controlled by a dielectric discharge barriers for UV light emission
Sara Saidi	Analyse électrique et cinétique d'une source plasma de photon dans le mélange Ne/Xe
N.Ait Hammouda	Development and study of UV lamps in the 207 nm for biomedical applications

Nom et Prénoms	**Session Poster RM** Modeling and simulation of radiation-matter interaction
Rachid Djeffal	Energy efficiency issues for the development of different climate sites
Maroc Fatima Zohra	Study of the physical characteristics of sodium halides in interaction with X-rays

Nom et Prénoms	**Session Poster NMM** New magnetic materials & Optoelectronic materials
Mardhi Lina	Numerical simulation of the effect of temperature on the performance of a GaSb-based TPV cell
Arbia Cheriet	Effect of defects on the performances of a TPV cell using InAsSb as active material
Imene Aouad	Electrical and optical behavior of an InAsSb based nBn structure for infrared conversion

Responsible (Pr)	Research areas	Code
H.Alla	Enhanced Oil Recovery (EOR) and Reservoir Simulation	EOR-RS
M.Abdelouahab	Fluid Mechanics : Two-phase flows	FM
M.Ferhat & B.Bouhafs	New materials for renewable energies (Photovoltaic, thermoelectricity, energy storage (battery), …): Modeling (First principle study) and Design.	NME
M.Adnane	Nanostructures and Nanomaterials	NNM
M.Elchikh	New magnetic materials	NMM
S.Hiadsi	Optoelectronic materials	OM
S. Bendella	Plasma and energy conversion	PEC
N.Belkaid	Modeling and simulation of radiation-matter interaction	RM
A.L.Khelil	Modeling and analysis of COVID-19 epidemics with treatment	CE

2 Conference Presentation

Dear Researchers and Colleagues,

It is a great pleasure to announce that the Committee of the Material Physics and Fluids Laboratory will host the national Conference on Material Physics and Fluids (CPMF-2022) which will be held in the prestigious city of Oran (Algeria) on December 12 to 14, 2022. The CPMF-2022 Conference aims to bring together renowned researchers and scientists to exchange ideas, to present relevant research work, to discuss hot topics in the field, and also share their experiences on all aspects of Material Physics and Fluids.

WHO predicts that the coronavirus pandemic will not end in 2022, so we have great confidence to launch the Conference on Material Physics and Fluids (CPMF-2022), which will be held on December 12-14, 2022 at the Andalouses complex, Oran, Algeria. On behalf of the committee, also we sincerely invite our research scientists in the respective fields to act as a speaker/chairman to give a lecture on the coronavirus pandemic.

We look forward for the participation of most researchers from all universities and research centers throughout the national territory.

3 Scientic committee

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5 Enhanced Oil Recovery (EOR) and Reservoir Simulation

5.1 Plenary Session

Chemical Product Design Methodology applied to Formulated Products and Enhanced Oil recovery EOR

Thibault Roques-Carmes[1,*], *Dayan* L Buitrago-Rincon[1,2], *Cécile* Lemaître[1], *Ronald* A Mercado[2], *Julio* A. Pedraza-Avella[2], *Philippe* Marchal[1]and *Véronique* Sadtler[1]

[1] 1Laboratoire Réactions et Génie des Procédés, Université de Lorraine, France
[2] 2Grupo de Investigación en Fenómenos Interfaciales, Reología y Simulación de Transporte (FIRST), Universidad Industrial de Santander, Bucaramanga 680002, Colombia

Abstract. Recently chemical product design has emerged as an innovative approach to develop new chemical and formulated products with targeted end-used properties based on consumer needs. The approach includes the process and chemical engineering aspects (agitation, mixing, reactor design, etc), the formulation by the choice of ingredients (powders, oil, water, surfactants, polymers, etc) and the physicochemical properties especially at the interfaces. In this lecture, the methodology will be presented stressing the multi-scale and multidisciplinary approach as well as the reverse methodology. The methodology will be then applied to complex fluids such as Pickering emulsions and enhanced oil recovery. Pickering emulsions are a peculiar type of emulsions for which the droplets are stabilized by the presence of nano or microparticles. This kind of emulsions appears as an alternative to classical emulsions stabilized with surfactants. Consequently, Pickering emulsions are becoming an attractive option during the development of innovative products when bio-based particles, polymeric particles, or biodegradable particles are considered. The chemical product design methodology is successfully applied to probe the repartition of the particles. The multiscale and multidisciplinary approaches are developed using several methods such as interfacial rheology, rheology of the emulsion, confocal microscopy, granulometry and mass balance approaches. The results indicate that the initial wetting of the particles, i.e. the particle dispersion in oil or in aqueous phase, the emulsification process (batch, semi-batch), the mode of mixing (rotor stator homogenizers or ultrasonic dispersers), the amount of dispersed phase, and the nature of the oil have an impact on the repartition of the particles. We demonstrate also that the rheological properties at the interface of the droplets are linked to the rheological properties of the emulsion and also to the texture, flow, stability and emulsification properties. Based on the results, the reverse engineering can be envisaged by tuning the wetting, the process, the interfacial properties and the formulation in order to reach the targeted end-used properties

Keywords: .

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Two-phase flowin macro and microchannels

Yacine SALHI[1,*]

[1] 1University of Sciences and Technology Houari Boumediene USTHB, Faculty of Physics Laboratory of Theoretical and Applied Fluid Mechanics, LMFTA, BP 32 El Alia 16111 Bab Ezzouar, Algiers, Algeria

Abstract.
Two-phase flow in both macro mini and microchannels has attracted people's concerns because of its wide applicability to advanced science and technologies such as micro-electro-mechanical systems, cooling of electronic components, bioengineering compact heat exchangers, chemical separation processes and biomedical systems. One of the issues to be addressed is whether or not two-phase flow patterns in microchannels are different from those encountered in ordinarily sized tubes. The flow structure of microchannel flows differs significantly from that observed in mini and macrochannels evenif the flow regimes are classified under the same name, some slight differences in the flow patterns can be observed between the macrochannels and the microchannels. The effects of surface tension are much more important in microchannels than those present in macrochannels. Hence, when classifying the flow regimes observed in a microchannel, both the effects of surface tension and the effects of inertia have to be considered. Despite of decades of attention and focus, whether from theoretical or experimental investigations, there is a lack of knowledge in the field of the two-phase flow in such small tubes [1].

Keywords: Two-phase flow, Macroscale, Microscale, Transition, Pattern

References

[1] Yacine SALHI

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Simulating vapour nucleation at nanoscale through diffuse interface modeling

Marco MARENGO[1,*]

[1]Advanced Engineering Centre, University of Brighton, Lewes Road, BN2 4GJ, Brighton, UK.

Abstract.
The prediction of the nucleation rate of vapour is a very difficult challenge. It depends on many factors which are complex and engaged: liquid and wall temperature, pressure, surface characteristics. Also the value of temperature of boiling onset is very difficult to be determined a priori, and in many cases it remains a tuning parameter for the CFD simulations. Presently, molecular dynamics is the only universally trusted tool to let the nuclei spontaneously appear, capturing the proper statistical properties. However, it can be used only for synthetic or particular fluids and has enormous computational cost limits. An alternative approach based on the coupling of Fluctuating Hydrodynamics Theory and Diffuse Interface modeling is possible. This approach gives access to mesoscale systems (up to 1 micron cube) at a much cheaper computational cost, and it enables the spontaneous nucleation of vapor bubbles in metastable quiescent liquid, thanks to the proper description of thermal fluctuations. The aim of the talk is to show the ability of this novel approach to numerically analyse the boiling inception phenomenon, addressing the detailed mechanisms underlying the vapor bubble formation, and gaining new insights for the surprisingly low superheat level measured in the experiments on ultra-smooth surfaces [1].

Keywords: CFD, Mesoscale systems, Boiling inception phenomenon, Vapor bubble.

References

[1] Prof. Marengo is a Physicist, Distinguished Professor of Thermal Physics at the University of Pavia

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5.2 Oral session

5.2.1 *Design of the chemical EOR by numerical solutions adapted difficult conditions of the reservoir in Algeria*

Design of the chemical EOR by numerical solutions adapted difficult conditions of the reservoir in Algeria

Hanène ZAHAF[1,*], *Hichem* BENAISSA[1] and *Hocine* ALLA[1]

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Abstract.
As Algeria's production capacities are expected to increase significantly in the short, medium and long term, the use of innovative oil recovery techniques has become increasingly important. One of the challenges in the design of chemical EOR is to develop chemical formulations and numerical solutions adapted to the difficult conditions of the reservoir in Algeria such as high temperature, high pressure and salinity for enhanced recovery objectives. As part of our present work, we study the flow of a chemical formulation on a porous medium, represented by oil field cores. According to the Ansys Fluent calculation code, the initial oil recovery rate can be predicted assuming that saturated oil exists in the medium. The purpose of our contribution, which introduces the CFD (Computational Fluid Dynamics) tool, is to understand the physical phenomena involved in the flow of chemical mixtures in cores. It consists of studying the effect of surfactant on the volume of fraction to the core outlet. This is the behavior of oil saturation as a function of space and time during flow. The results obtained require, to decide on the choice of the chemical formulation, more than real and reliable physical data on the wellbore, the production history, the geophysics of the terrain to be explored, the conditions of the reservoir, the real distribution of pores and the permeability of the medium, etc. It is wise to pronounce that this work will be used as support for the numerical study on the EOR. In the presence of the various data recorded, by the various services of the Algerian oil industry through qualified and professional personnel, the continuation of this work may lead to the affirmation of the choice of the surfactant, the operating mode to be undertaken, the risks related the methods used, etc., in the field exploitation of oil fields, within the framework of tertiary oil recovery [1].

Keywords: EOR, CFD, chemical flooding, PVT.

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Numerical simulation of CEOR processes - case studies.

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Abstract.
Oil production is separated into three phases: primary, secondary and tertiary, the latter is also known as Enhanced Oil Recovery (EOR). There are three main types of EOR, including chemical flooding, gas injection and thermal recovery. Since, EOR methods increase the cost of development of the hydrocarbons brought to the surface, producers do not use EOR on all wells and reservoirs. The economics of the development equation must be considered. Consequently, each field must be heavily evaluated to determine which type of EOR will work best on the reservoir. This is done through reservoir characterization, screening and reservoir modeling and simulation [1].

Keywords: EOR, Surfactants, Oil, Water, Gas, Permeability, Wet ability, Capillary pressure, Mobility.

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Molecular Dynamics simulation of the injection of polymer chains into a nanopore for enhanced oil recovery operation

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Abstract.
Extracting oil from porous underground formations is a complicated operation. Polymer injection into nanopores is a promising method for enhanced oil recovery (EOR). Understanding the molecular mechanism of polymers allowing the extraction of residual oil in nanopores is of great importance for the advancement of aging oilfields. In this work, we performed molecular dynamics simulations to investigate the process of oil extraction from a nanopore using a polymer chains. We found that the interactions between the polymer chains and oil provide better extraction of the residual oil confined in the nanopore and our results are in good agreement with the literature. This plays a key role in the amount of residual oil extracted in EOR operations [1–3].

Keywords: Molecular Dynamics, Polymer chains, Nnanopores-EOR

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Evaluation of the Effect of Polymer Flooding on Increasing Oil Recovery and Reducing Barrel Cost

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Abstract.
This work consists of an evaluation of the effect of chemical enhanced oil recovery by polymer injection on the improvement of oil recovery and the reduction of incremental barrel cost compared to water flood. Polymer flooding is an effective method to recover unswept oil in water injection processes by improving the mobility ratio. A simulation study was carried out in an Algerian reservoir with 3 scenarios; natural depletion, water injection and polymer injection, the oil recovery and the water cut for each scenario are compared. The main objective is to model and simulate the polymer flooding with sensitivity on the concentration of polymer and the volume of polymer injected. The implementation of polymer injection process as a secondary or tertiary recovery phase was also analyzed. A considerable improvement in the oil recovery by polymer injection was observed from the second phase of recovery, the cost of the barrel is reduced in the case of polymer flood compared to water flood, the effect of reducing the water-oil separation cost due to water-cut reduction was more important than the additional chemicals costs [1–4].

Keywords: EOR, Polymer flood, Reservoir simulation, Oil recovery.

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Performances & uncertainties of the chemical EOR process on the simulation model of Algerian field

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Abstract. Performing surfactant-polymer (SP or ASP) type chemical injection under very difficult conditions of high salinity (~237000 ppm) and high temperature (~120°C) presents a huge challenge. This challenge is related to the thermal stability of polymers at high temperatures, to the compatibility of surfactants with a high concentration of divalent cations present in the injection brine (~325 ppm). Recent work on that field has led to the determination of a new chemical formulation and a new polymer with moderate surfactant retention, an essential requirement for low chemical cost. Several formulations have been implemented and tested; exhibiting good solubility and compatibility with the polymer, thermal stability in reservoir conditions, ultra-low interfacial tension with good temperature robustness and good injectivity in the reservoir rock. Field applications of the CEOR process are challenging due to many uncertainties that can potentially impact project success. This even if the effectiveness of the chemicals injected are tested and validated in the laboratory. These uncertainties include chemical adsorption, residual oil saturation reduction by chemical injection, interfacial tension, capillary number, permeability reduction, inaccessible pore volume, and reservoir heterogeneity. This work focused on the investigation of the impact of the variation of the most uncertain chemical parameters on the chemical performance, the gain in cumulative oil production as well as the economic viability of the chemical EOR process.

Keywords: Modeling & Simulation, chemical flooding methods, reservoir, enhanced recovery, Chemical EOR Uncertainty , slug size, residual oil saturation, surfactant adsorption, oil price, chemical cost..

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5.3 Poster

5.3.1 *Green and rapid extraction of essential oil from Algerian Origanum majorana*

Green and rapid extraction of essential oil from Algerian Origanum majorana

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Abstract.
the aim of this work was to determine the chemical compositions of essential oils of dried Origanum majorana leaves and to characterize thier antibacterial activities using a disc method. The origanum majorana essential oils were isolated by hydrodistillation (HD) and microwave assisted extraction (MAE). A total of 16 and 15 constituents were identified by GC/MS, obtained by HD and MAE, respectively; the main components detected were: terpin-4-ol(20.02%, γ-terpinene (14.61%), α-terpinene(5.11%), α-terpinene(3.45%) and sabinene(2.53%). Origanum majorana essential oils were tested for thier antimicrobial activity against four bacteria strains (S. aureus ATCC 29213, S. aureus, E. coli MA and K. pneumoiniae). the origanum majorana oils showed a good antimicrobial activity against all Gram (-) and Gram (+) bacteria for both extraction methods. Antibacterial activities were correlated to the chemical compositions of the essential oils. Finally, the dried origanum majorana leaves have a potential source of natural antimicrobial, it can be suggested to use thier essential oils as potential natural preservatives and would be helpful in the treatment of various infections.

Keywords: Essential oil, Hydrodistillation, Microwave assisted extraction, Dried Origanum majorana leaves.

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Improved of enchanced oil recovery by injection of surfactant polymer

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Abstract.
In order to increase oil recovery beyond primary and secondary recovery, manufactures practice Enchanced Oil Recovery (EOR) process that consist of the injection of fluids other than water into the oil reservoir. Such that it is estimated to recover approximately 65% of the initial oil in place (OOIP) remaining in the after secondary recovery. The increasing value of EOR in the word, made possible by the report of new technologies, is exactly argued by the large quantity to be recovered [1]. In conventional methods, also khown as secondary recovery, water or immiscible gas is used as the working fluid. Another phase of recovery, called enchanced or terciary, intervenes further to improve oil production. In this process recovery, the injection of polymer solutions is the most technique used, especially for heavy oils. The effectiveness of this method is attributed mainly to the reduction in the mobility of the aqueous phase and the viscoelasticity of the polymers. Enchanced Oil Recovery (EOR) processes are defined to include processes that increase oil recovery beyond secondary recovery. They are defined by the injection of surfactants, in which the behavior of a phase inside the reservoir can be manipulated. All surfactant systems, and crude oil create micro-emulsions at the interface between crude oil and water, with limits for the reduction of interfacial tension down to an ultra-low value (0,001 mN/M) and automatically the residual oil will be mobilized in the tertiary recovery [2]. The objective of our work is to study the measures and injection methods of surfactants and polymers to improve the recovery of oil from the reservoir

Keywords: EOR, Surfactant, emulsion, Demixing.

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6 Fluid Mechanics (FM)

6.1 Plenary Session

6.2 Oral session

6.2.1 *Numerical simulation of blood flow in the bifurcation of the carotid artery*

Numerical simulation of blood flo wi nthe bifurcation of the carotid artery

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Abstract.
In this work, the blood flow in the carotid artery bifurcation was studied by numerical simulation, and this was done using the commercial program, a numerical simulation of Newtonian and non-Newtonian fluid (Carreau-Yasuda and Cross model) was performed in the carotid bifurcation of Reynolds number Re = 151 (peak Systole) and Re = 377 (peak diastole). The effect of fluid behavior a nd Reynolds number on the field of velocity, viscosity, and pressure was shown. The study confirmed the presence of secondary flows within the internal carotid artery in the sinus region. Note that the latter is characterized by the presence of blood particles opposite rotation responsible for the narrowing in the artery

Keywords: Blood flow ;Carotid bifurcation ;Recirculation ;Shear-thinning fluid.

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Hydrodynamic performances of non-Newtonian fluid mixing in passive microfluidic devices

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Abstract. High mixing performances micromixers are widely used in various industrial applications. Mixing in the laminar regime and at low Reynolds numbers is of major importance in some processes. The implementation of the physical phenomenon of chaotic advection to improve mixing efficiency is a known technique. Therefore, the secondary flows resulting from this phenomenon are very intense and act at the microscopic level during homogenization. This study aims to compare different configurations of passive micromixers. The four micromixers examined are successively: Two Layer Crossing Channel Micromixer (TLCCM), Semicircular Serpentine Micromixer (SCSM-90), Curved micromixer with Grooves (CG), and C-Shape micromixer. All micromixers have the same hydraulic diameter and the same unfolded length. Numerical simulations were performed at low Reynolds numbers using the CFD Fluent code. The shear-thinning fluids used are CMC solutions which are modeled by a power-law model with a power-law ranging from 0.73 to 1 and the generalized Reynolds number varies between 0.1 and 50. The mixing efficiency was evaluated by calculating the mixing index (MI) in different cross sections. To analyses the obtained results through the numerical simulations, the mass fraction distributions, the velocity vectors and profiles and the pressure drops have been presented in different cross sections. The obtained results show that the TLCCM micromixer has the highest mixing index which exceeds 0.96 for all values of generalized Reynolds number and the considered power-law index, it also has the lowest mixing energy cost compared to other micromixers

Keywords: Chaotic advection; Non-Newtonian fluids; power-law index; Mixing index, Mixing Energy Cost.

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Numerical simulation of the creation and diffusion of a vortex ring in a non-Newtonian fluid

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Abstract. The numerical investigation of the formation and growth of a vortex ring in diverse fluids (shear thinning, viscoelastic and viscoplastic) with low Reynolds numbers will be carried out using CFD (Computational Fluid Dynamics). The numerical model will be validated by comparing the data to those produced by PIV at the IMFT (Institute of Fluid Mechanics Toulouse) [3]. Many experiments and numerical study have been conducted in Newtonian fluids with high Reynolds numbers [1, 2]. The goal of this work is to extend it by investigating the impact of different non-Newtonian structures on the global dynamics of the vortex. Then, at extremely low Reynolds numbers, the impact of geometric factors on the dynamics of the vortex is investigated

Keywords: Vortex ring, Vorticity, CFD.

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Numerical study of the motion of a solid particle carried by a gas in a micrometric system

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Abstract. Nowadays, the fumes and harmful gases escaping from factories and means of transport have reached a very high rate, which has become worrying since the latter are loaded with particulate matter (PM) which causes serious health problems. The danger of these PMs, in addition to their toxicity, comes from their microscopic size, which allows them to penetrate deep into the lungs, and some can even enter the bloodstream. On the other hand, research on Micro-Electro-Mechanical Systems (MEMS) in general and microfilters, in particular, has made great progress because they represent effective devices to fight against these PMs by detecting, trapping, and neutralizing them. In this work, we are interested in studying numerically, using the COMSOL software, the movement of solid particles carried by gas through a microchannel, the flow is due to the pressure gradient and the temperature is considered constant. The study is carried out for particles of different sizes and densities. While taking into account the rarefaction of the flow

Keywords: Rarefaction, particulate matter, microchannel, drag force, microfluidic.

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Hydrodynamic performances of non-Newtonian fluid mixing in passive microfluidic devices

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Abstract. High mixing performances micromixers are widely used in various industrial applications. Mixing in the laminar regime and at low Reynolds numbers is of major importance in some processes. The implementation of the physical phenomenon of chaotic advection to improve mixing efficiency is a known technique. Therefore, the secondary flows resulting from this phenomenon are very intense and act at the microscopic level during homogenization. This study aims to compare different configurations of passive micromixers. The four micromixers examined are successively: Two Layer Crossing Channel Micromixer (TLCCM), Semicircular Serpentine Micromixer (SCSM-90), Curved micromixer with Grooves (CG), and C-Shape micromixer. All micromixers have the same hydraulic diameter and the same unfolded length. Numerical simulations were performed at low Reynolds numbers using the CFD Fluent code. The shear-thinning fluids used are CMC solutions which are modeled by a power-law model with a power-law ranging from 0.73 to 1 and the generalized Reynolds number varies between 0.1 and 50. The mixing efficiency was evaluated by calculating the mixing index (MI) in different cross sections. To analyses the obtained results through the numerical simulations, the mass fraction distributions, the velocity vectors and profiles and the pressure drops have been presented in different cross sections. The obtained results show that the TLCCM micromixer has the highest mixing index which exceeds 0.96 for all values of generalized Reynolds number and the considered power-law index, it also has the lowest mixing energy cost compared to other micromixers

Keywords: Chaotic advection; Non-Newtonian fluids; power-law index; Mixing index, Mixing Energy Cost.

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6.3 Poster

6.3.1 *Parametric study of the effect of the crossing elongation on the mixing performances of a compact microfluidic system*

Parametric study of the effect of the crossing elongation on the mixing performances of a compact microfluidic system

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Abstract. In this study, we invistigate the hydrodynamic mixing performances of a compact microfluidic system represented by a passive micromixer of the TLCCM type, which offers high mixing performances compared to other micromixers studied recently, our idea suggests a modification in the crossing zone to reduce the number of mixing units. Numerical simulations were performed at low Reynolds numbers using the CFD Fluent code. The elongation of the crossing zone is defined by a parameter called « aspect ratio » (l/W). A parametric study was realized using five values of aspect ratio from 0 to 1 in a wide range of Reynolds numbers: from 0.2 to 80. To analyze the obtained results, the mass fraction contours, the velocity vectors, the velocity profiles and the pressure losses were presented in different planes and positions. The selected micromixer (with l/W = 1) has the better mixing performances where the mixing obtained index exceeds 85.67% for Re = 0.2 and reaches 99.22% for Re = 50, it also has the lowest pressure losses compared to other micromixers studied recently. Therefore, the chosen micromixer exhibits high mixing performances at low Reynolds numbers, so it can be used to improve the mixing quality in the passive microfluidic systems

Keywords: Micromixer, TLCCM, CFD, Low Reynolds numbers, Chaotic advection, Mixing index, Mass fraction, Pressure losses.

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Numerical investigation of the hydrodynamic aspect of a liquid-liquid extraction column at various stirring speeds

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Abstract. Liquid-liquid extraction is a separation method based on the distribution of distinct separable components between two or more liquid phases. This approach is frequently used in industry and attempts to evaluate the parameters of hydrodynamics, instabilities, and transfer phenomena, as well as their effect on extraction quality and process time. The two-phase hydrodynamic flow in a liquid-liquid extraction column will be numerically studied in this work using CFD (Computational Fluid Dynamics). The goal is to investigate the hydrodynamic component and comprehend the current turbulence phenomena by adjusting the agitation speed. The computerized model will be validated by comparing the results to those obtained experimentally in a prior investigation on a liquid-liquid extraction column conducted by the PIV (Particle Images Velocemetry).

Keywords: Liquid-liquid extraction; CFD; two-phase flow; hydrodynamics; Turbulence.

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7 New materials for renewable energies (NME)

7.1 Plenary Session

7.1.1 *Cu-based Half-Heusler alloys for spintronic devices: ab-initio prediction of new stable phases*

Cu-based Half-Heusler alloys for spintronic devices: ab-initio prediction of new stable phases

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Abstract.
The structural, vibrational, elastic, mechanical, thermodynamic, magnetic and electronic properties of a series of Cu-based half-Heusler alloys in different α, β and γ configurations were investigated using first-principles calculations based on spin-polarized density functional theory using the generalized gradient approximation (GGA-PBE) for the energy and the exchange and correlation potential. The cubic ($F-43m$), hexagonal ($P-62m$, $P63mc$, $P63mmc$), tetragonal ($P4/nmm$), and orthorhombic ($Pnma$) phases of the half-Heusler CuXGe (X=Cr, Mn, Fe, Co, and Ni) alloys [1–3] were considered. From the various phases, we noticed that the most structurally stable phase for the considered alloys is non cubic. The elastic properties and phonon spectra calculated in different phases showed that the half-Heusler alloysare elastically and dynamically stable in different phases in correlation with the chosen transition element (Cr, Mn, Fe, Co, and Ni).

Keywords: DFT, Ferromagnetism, Phonon, half-Heusler, Transition element

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7.2 Oral session

7.2.1 Simulation of thin film solar cells of CIGS with AMPS-1D software

Simulation of thin film solar cells of CIGS with AMPS-1D software

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Abstract. In this study we explore the effect of thickness on the performance of copper indium gallium diselenide (CIGS) thin film solar cell has been numerically simulated with the AMPS-1D software for the simulation. The cell structure based on CIGS compound semiconductor as the absorber layer, In_2S_3 as a buffer layer, $ZnO : i/ZnO$ a sa window layer. This study aimed to find the optimum thickness of buffer and absorber layer for a CIGS thin film solar cells with indium sulfide buffer layer. It is found that the optimum thickness of the buffer layer is from 40nm to 50nm and for the absorber layer is in the range of 2000nm [1–3]

Keywords: Hydrogen production, Reaction mechanisms pathway, Dielectric barrier discharge, Conversion, Yield.

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Numerical modelling of ultrathin $Cu(In,Ga)Se_2$ solar cells

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Abstract. In this work we used the AMPS-1D software for the simulation of the high efficiency $Cu(In,Ga)Se_2$ (CIGS)-based solar cells solar cells. The first purpose in this paper is deal with the influence of various thicknesses of CIGS layer on the performance of the CIGS-based solar cells. The photovoltaic parameters have been calculated with different variation of 300 *nm*-1000 *nm* for $CuIn_{1-x}Ga_xSe_2$ absorber layer thickness. Results show that the performance of CIGS solar cells decreases as the absorber layer thickness is decreased Conversion efficiencies decreases by 4 %. In the second par to four works, we studied the effect of incorporation of band gap grading or commonly known as back surface field in the ultra thin CIGS solar cells which improve the performance of the cells. For the graded cells, efficiencies of 12.38 % and 17.26 % are achieved for cells with 300*nm* and 1000*nm* thick absorber layers. These improvements are attributed to the less recombination loss at the $CIGS/Mointerface$ [1, 2].

Keywords: CIGS, BSF, AMPS-1D, Band gap grading, Thin film solar cells.

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Defect density influence of the crystalline silicon for the structure $ITO/a: Si-H/c-Si/Al$ in the dark and under illumination

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Abstract. Sometimes the bad cleaning of crystalline silicon causes the presence of defects [1], these defects may present in the middle of the energy band of crystalline silicon by a continuous variation of the defects densities NT. In this work we show the influence of the crystalline silicon defects densities for the structure $ITO/a: Si-H(p+)/c-Si(n-)/Al$ on the electrical characteristics in the dark and the photovoltaic parameters under illumination through SCAPS simulation software. The study in darkness shows that conduction and assisted by at least two conduction mechanisms, and the operation of the electrical characteristics $Ln(I)-V$ shows that the absence of defect density in crystalline silicon results from a single slope or a single conduction mechanism. On the other hand, the presence of defects causes two slopes, which means two conduction mechanism. The ideality factors range from $1.94-1.08$ to $N_T = 8.10^{13}\ cm^{-3}$ up to $2.02-1.22$ to $N_T = 8.10^{14}\ cm^{-3}$ successively for the first and second slopes, saturation currents $10^{-9}-5.10^{-15}$ to $N_T = 8.10^{13} cm^{-3}$ up to $2.10^{-8}-1.2210^{-11}$ $A.cm^{-2}$ at $N_T = 8.10^{14}\ cm^{-3}$ successively for the first and second slopes. Those results proved that the recombination generation mechanism and the diffusion or thermo ionic mechanism are responsible for the conduction At under illumination, the linear characteristic I-V has a better form when the density N_T decreases and the maximum power decreases according to the density N_T of the amorphous layer. Whenever the density N_T increases and the I-V characteristics degraded [2]. And finely the output parameters V_{co} , I_{CC}, $FF\eta$ of the solar cell decrease with the increase of the defect density N_T, the absence of defect density in crystalline silicon the yield is around to 14 %, the yield value is 2.7 % with density $8.10^{13}\ cm^{-3}$ and minimum yield and order 5.7% with density $8.10^{14}\ cm^{-3}$.

Keywords: Amorphous silicon, Crystalline silicon, Defect densities, Conduction mechanisms .

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Organic MA cation A-site doping in $CsPbI_3$ perovskite by first principle calculations

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Abstract. The metal halide perovskite $CsPbI_3$ is one the most important scientific discoveries in the field of optoelectronics and photonic devices, especially solar cells [1, 2]. Its commercial application is hindered by the fact of instability. In order to overcome the instability of the compound, we have doped A site CsPbI3 cation with organic MA $(CH_3NH_3)^+$ [3, 4]. Using first principle calculations within density functional theory, we have calculated thermodynamic, structural, electronic and optical properties of both all-inorganic and $(CH_3NH_3)^+$ doped $CsPbI_3$. Our calculation results indicated that $Cs_{0.5}MA_{0.5}PbI_3$ has formation energy value lower than the undoped $CsPbI_3$ which mean that doping A-site organic cation might improve the stability of the compound and also make the band gap adjustable. These properties can provide research ideas for subsequent research of A-site doping organic cations.

Keywords: Density functional theory , organic inorganic perovskite, optical properties.

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First-principles study of structural, electronic, magnetic properties and elastic anisotropy of $Sr_{1-x}TM_xS$ (TM = Fe, Co)

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Abstract.
We have performed first-principles calculations in order to investigate the electronic structure, the magnetic, the elastic constants, the mechanical properties, the lattice-dynamics and the thermodynamic properties of rubidium and cesium sulfides RbS and CsS in the CsCl (B2) phase. Features such as equilibrium lattice constant, bulk modulus, spin-polarized electronic band structures, total and partial densities of states, elastic constants and magnetic properties are calculated. using the full potential linearized augmented plane wave approach to the density functional theory within generalized gradient approximation (GGA) for the exchange and correlation energy. Total energy calculations are also carried out using the pseudopotential method, which allowed us to investigate the phonons dispersion spectra and the total and the partial phonons densities of states (PhDOS) from the linear-response of density-functional theory. Some fundamental thermodynamic properties and their variation with temperature are also calculated in the framework of the quasiharmonic approximation such as heat capacity, entropy, internal energy, free energy of vibration, and mean squared displacement (MSD). The studied compounds RbS and CsS in the CsCl structure are found to be half-metallic ferromagnets with 100 % spin polarization at Fermi level EF. Therefore, these materials are suitable candidates for application in spintronic devices [1, 2].

Keywords: First-principles, Electronic structure, Phonon, Thermodynamic properties, Half metallic ferromagnetism.

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Ab-initio study of the electronic structure of Barium Oxide BaO and the $NaBa_3O_4$ alloy

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Abstract.
In this work, by performing first-principle self-consistent calculations, the structural and electronic properties of the Barium Oxide compound BaO are studied in three different structures; the cubic $Fm\bar{3}m$ structure, the hexagonal $P63mmc$ structure, and the tetragonal $P42mnm$ structure. A direct gap in X of 4.1 eV was found in the cubic structure, wich is in a good agreement with experimental results [1, 2], while for the other two structures the gaps are indirect. Thermodynamic stability is verified by calculating the enthalpy of formation ΔH, in both the cubic and hexagonal phases. Analysis of the calculated elastic constants and phonon dispersion curves reveals that all phases studied are mechanically and dynamically stable.Subsequently, BaO is doped with the element Na (belonging to the alkali metal family), thus forming the alloy $NaBa_3O_4$. A comparative study of the ferromagnetism and non-magnetism of this alloy is undertaken. All structural, electronic, mechanical and dynamic properties are studied in the simple cubic structure $Pm\bar{3}m$. This study reveals the ferromagnetic stability of this alloy

Keywords: Barium oxide, Ferromagnetism, Half metallicity

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Development of selective emitter solar cells with LASER doping

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Abstract. P-type solar cells are being developed as next generation photovoltaic solar cells, and have attracted a significant amount of attention [1]. In addition, the demand for high-efficiency silicon solar cells has increased in order to reduce production costs and save space [2]. In this study, we demonstrate the formation of selective emitter through laser doping (LD) [3, 4]. Si wafer totally diffused emitter ($60\Omega/sq$) by LYDOP diffusion technique. The sheet resistance was ($30\ \Omega/sq$) at the local phosphorus emitter after LD. The phosphor diffusion depth was $\backsim$ 0.8-1 μm , and the phosphor surface concentration was $7 \times 10^{19}\ atoms/cm^3$. The p-type solar cells were fabricate dusing phosphor LD to have front side phosphor selective emitters. The characteristics of the newly developed solar cells improved in comparison with those of the reference cells (i.e., those without boron selective emitters). The improved efficiency was mainly due to the increase in the short circuit current density and fill factor.

Keywords: Solar cell, Laser doping, Selective emitter.

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Optimisation of the photovoltaic efficiency of a cell based on GaAs

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Abstract. Photovoltaic solar energy is a direct transformation of part of the solar radiation into electrical energy. This energy conversion is carried out by means of a solar cell whose efficiency depends on the range of the solar spectrum absorbed.Nowadays, thin-film solar cells are increasingly used mainly because of their low cost. This work consists in simulating and modeling a solar cell based on the GaAs material. The simulation was carried out by the mathematical tool Matlab. For this we have considered a GaAs-based cell already in theoretical and experimental study. The latter had a rate of return of 18.5 % in theory and 19 % in experimental [1]. Taking into account the ideal conditions of T=298 K and solar intensity of 1000 W/m^2, we have achieved a yield that is worth 19.2%, a value close to that obtained in experiments. Outside, to deepen in the simulation, we considered a variation of some parameters that seemed to influence the characteristics of the cell such as: coefficient of absorption, density of electrons and factor of ideality. We have proceeded in such a way that each time we vary one parameter the other two are considered constant. For this, the influence of the factor of ideality with a value higher than that of the theory, led us to a higher yield of 25.5 %. Therefore, by increasing the value of the coefficient of absorption, the value of yield fell by 20.1 % compared to the influence of the factor of ideality but a value superior to the theory. Let us end by the influence of the density of electrons, or the decrease of the latter generates an increase in the efficiency that was worth 21.3 % compared to the theory.The results obtained allowed us to model a cell based on GaAs with a yield of 29.8 %. Then our simulation continued with a real study whose temperatures and solar intensities are those of January and December for the year 2021 in the Tlemcen region. Or yield to slightly decrease to become 24.3 %.

Keywords: photovoltaic, solar cell, GaAs, simulation, materials.

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PERFORMANCE OF A MICROBIAL FUEL CELL : APPLICATION OF RENEWABLE ENERGIES

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Abstract. A Microbial Fuel Cell (MFC) was conceived by using garden soil as a source to culture. It was then utilized as a bio-catalyst to decompose waste organic matter, reduce pollution from the soil, and produce energies. The MFC was composed of a bio-anode inoculated with a mixture of garden compost leachate and an abiotic stainless steel cathode. Besides, the bio-anode consisted of a Nafion membrane modified with carbon. The microorganisms agglomerated under polarization and formed electroactive bio-film onto bio-anode. In the preliminary test of MFC, potassium hexacyanoferrate has been utilized as catholyte, to enhance the reduction of proton and electrons resulting in a higher voltage. However, this electrolyte is toxic and oxidized rapidly, thus substituted by the hydrochloric acid. The results showed that the MFC with modified Nafion, gave relatively high current-density 379 mA/m2 in two days, whereas the conventional biofuel cell without modification attained the current-density 292 mA/m2 in four days. Nevertheless, both cells yielded almost the same current density of 20 mA/m2 during 60 days. Although it has been used for a long time, the modified Nafion has not been corroded and preserved its physicochemical properties.

Keywords: microbial fuel cell; garden soil leachate; Nafion117 membrane; carbon powder; surface modification; bioenergy; electrochemical characterization.

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First-principles study of the Heusler superconductors Ni_2ZrX (X= Ga and Al)

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Abstract. In this work, a theoretical study was carried out on some physical properties of Heusler alloys Ni_2ZrX (X = Ga and Al) in the both regular and inverse structures. The pseudo potential approach was used within the framework of density functional theory which is implemented in the Quantum Espresso calculation code. The exchange and correlation potential was addressed by the generalized gradient approximation (GGA-PBE). The Cu_2AlMn-type structure is found to be energetically more favorable than the Hg_2CuTi-type structure for the both compounds. The occurrence of superconductivity was confirmed for these compounds using electronic structure calculations.

Keywords: Ni_2ZrAl, Ni_2ZrGa, DFT, Heusler superconductors, Quantum Espresso.

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First-principles study of optoelectronic properties of Cu-based chalcogenides

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Abstract. Kesterite and Stannite Cu_2ZnSnS_4 (CZTS) semiconductors are potential solar absorbing materials [1-3]. They have been widely studied in recent years due to their advantageous properties, including terrestrial abundance of its constituent elements, non-toxicity, suitable bandgap. Using first-principles calculations based on density functionnal theory (DFT), the electronic, optic and dynamyc proprieties are studies. In our work we have extended our study of this material in the orthorhombic phase, the calculation of the band gaps carried out using (GGA+U) [4], the values of the gaps obtained are in very good agreement with the experimental values, and which are equal to 1.30, 1.264 and 1.374 eV in Stannite, Kesterite and orthorhombic structures respectively. We also calculated the yield according to the thickness and which is of the order of 32.35%, 31.95% and 32.34% in the Stannite, Kesterite and orthorhombic phases respectively.

Keywords: Cu_2ZnSnS_4, Photovoltaic, DFT.

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Investigation of Various Properties of Anti-perovskite Based Rare Earth AlNS c3

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Abstract. In this report, we present the results of ab initio calculation of anti-perovskite ni trides based rare earth AlNS c3. The structural and mechanical properties were calcu lated using FP-LAPW method [1], the elastic results are proved the mechanical stability of this compound, our finding results are in good agreement with available results. More over, we have studied the dynamical stability of AlNS c3 compound using QUANTUM ESPRESSO package (QE) [2, 3] within PP-PW approximation. The positive frequen cies of vibration modes are obtained and which confirmed the dynamical stability of the present alloy.The electronic band, total and partial density (DOS+PDOS) curves of anti-perovskite AlNS c3 are plotted and discussed, the electronic nature of the studied material is metallic behavior

Keywords: Antipervskite, AlNS c3, FP-LAPW and PW-PP, dynamical stability.

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Mixed halide perovskite for solar energy conversion, Alloys and their effect on material stability

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Abstract. Inorganic perovskites materials are very promising compounds as solar cells absorber layer, due to their higher stability then organometallic perovskites [1]–[5]. In order to stabilize the preferred black phase perovskite crystal structure at lower temperature. $CsPbI_3$, $CsPbBr_3$ and their alloys are studied and show promising results[6], [7]. Indeed, we employ the pseudo-potential plane wave approach as implemented in the Quantum ESPRESSO code to comprehensively examine the structural, electronic, and mechanical properties of these perovskites materials. The mechanical characteristics indicate the stability, flexibility, and softness of both compounds and their solid solution and all results are in good agreement with available experimental and theoretical results.

Keywords: Halide perovskite, perovskite solar cell, Alloys, DFT.

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Doping and co-Doping Impact on the Structural, Electronic and Magnetic properties of CeO_2 : based on first principle calculation

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Abstract. We report the effects of doping with Magnesium (Mg) and co-doping with Magnesium and Titanium (Mg , Ti) within Cerium dioxide containing weight ratio 12.51 to replace Ce atom. The changes, due to the doping and co-doping , in structural, electronic and magnetic were studied. Full Potential Linear Augmented Plane Wave (FP-LAPW) method based on Density Functional Theory (DFT) is implemented. We used both WC-GGA [1, 2] and TB-mBJ exchange-correlation functional [3] in solving Kohn-Sham equation as incorporated in the WIEN2k code [4]. As results after substitution of atoms, our computed lattices parameters for $Ce_{0.875}Mg_{0.125}O_2$ and $Ce_{0.750}Mg_{0.125}Ti_{0.125}O_2$ equal to: (10.75 Å , 10.63 Å) respectively , the volume optimization predicts that the compounds are more stable in ferro-magnetic phase. The compounds of $Ce_{0.875}Mg_{0.125}O_2$and and $Ce_{0.750}Mg_{0.125}Ti_{0.125}O_2$ were formed which favor half-metallic ferromagnetism . This stady play a vital role in increasing the magnetic moments of the super cells. Calculated results indicate that the electronic and magnetic properties provide a new route to the experimentalist for the potential applications in spintronic devices.

Keywords: FP-LAPW , Wien2k , TB-mBJ , co-doping , half-metallic , spintronic.

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7.3 Poster

7.3.1 Ab initio calculations of the fundamental properties of half-metallic materials : Possible Candidates for modern spintronics devices

Ab initio calculations of the fundamental properties of half-metallic materials : Possible Candidates for modern spintronics devices

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Abstract. The fundamental properties of $Sr_{1-x}Ti_xSe$ and $Ca_{1-x}Cr_xSe$ ternary alloy are examined at concentration (0.25) in the rock salt (B1) phase.The calculations are performed using the full potential linearized augmented plane wave plus local orbital (FP-LAPW+lo) method[1] within the framework of the density functional theory (DFT)[2]and the generalised gradient approximation (GGA)The state stability of $Sr_{0.75}Ti_{0.25}Se$ and $Ca_{0.75}Cr_{0.25}Se$ have been investigated by calculating the variation in total energy versus volume for different magnetic states. It is verified that the stable state of all compounds is the ferromagnetic structure. Features such as the equilibrium lattice parameter and bulk modulus are measured too. The exploration of the energy band gaps, however, revealed that these compounds have direct gaps at $(\Gamma - \Gamma)$ direction of the spin down case. The electronic structures are found to present a half metallic ferromagnetic behavior for all compounds. The total magnetic moments value affirm the right ferromagnetic nature of the systems utilized. The integer value of the total magnetic moments of calculated compounds have been estimated to equal to 2μB and 4μB per Ti atom and Cr atom respectively. Therefore, the $Sr_{0.75}Ti_{0.25}Se$ and $Ca_{0.75}Cr_{0.25}Se$ ternary alloy seems to be a new potential candidate for modern spintronics devices[3, 4]

Keywords: DFT,FP-LAPW, spintronics, DMSs, structural properties.

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First-principle study of Physical properties of new half-metallic quaternary Heusler alloys: CoZrYP (Y=Mn and Fe)

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Abstract.
Now, the new challenge of the scientific community is to decrease energy consumption, Spin electronic or Spintronic devices [1,2] are the perfect example of this new orientation, The Spintronic devices use electron angular momentum, A prime example of the advantage of employing spin rather than electric charge is found in the newly developed magnetic random access memory (MRAM)[3, 4] which is proposed as a replacement for the dynamic random access memory (DRAM) [5] based on three-terminal metal-oxide-semiconductor (MOS) devices[6], Heusler compounds [7, 8] offer potential as spintronic devices due to their spin-polarization and half-metallicity properties[8, 9]. We focus on the study of robust half-metallicity of a new half-metallic quaternary Heusler: CoZrYP (Y=Mn and Fe)[10, 11], Using the first principle study we examined its structural, electronic and magnetic properties with the full-potential linearized augmented plane wave (FP-LAPW) method [12, 13] within the generalized gradient approximation (GGA) [14, 15]and the generalized modified potential plus Becke-Johnson approximation (GGA-mBJ)[16], The spin-polarized electronic density of states calculations show that CoZrYP (Y=Mn and Fe) compounds display a half-metallic behavior, with the majority spin being metallic and minority spin being semiconducting

Keywords: Quaternary Heusler, first principle calculations, half-metallic, spintronic.

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Structural, electronic, optical and thermoelectric properties of halide double perovskite Cs_2AgBiX_6 (X = F, Br): DFT study

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Abstract. A theoretical study of the structural, electronic optical and thermoelectric properties of halide double perovskite Cs_2AgBiX_6 (X = F , Br) by using the first principles density functional theory (DFT) calculations performed in the full potential linear augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [1]. Within the and generalized gradiant approximation (GGA) for potential exchange correlation [2]. is also used for calculating the electronic, optical and thermoelectric properties of the material We have analyzed the structural parameters, total and partial densities of states, Optical properties are discussed in terms of dielectric constants, absorption coefficients, refractive index and reflectivity. according to the electronic properties of these compounds, that they have a semiconductor moreover these compounds are characterized by a very important value of the factor of merit (ZT), electrical conductivity, thermal conductivity and the Seebeck coefficient, which make these compounds promising candidates for thermoelectric applications

Keywords: double perovskites, DFT,optical properties,thermoelectric properties, FP-LAPW.

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Approximations choice and adequate conditions for the investigation of ZnO properties

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Abstract. A renewable interest is shown for zinc oxide, ZnO, as a promising material for several potential applications in numerous fields due not only to its very good optical and electrical properties but also to its high chemical stability and its non-toxicity [1]. Thus, several experimental and theoretical approaches are being developed to determine its optimized properties [2, 3]. However, the choice the appropriate method and the adequate conditions to study this material still represents a great challenge to get accurate results in less investigation time. In this context, to overcome such difficulties, we adopted a simulation approach based on the use of the full potential linearized augmented plane wave (FP-LAPW) method, as part of the density functional theory (DFT). Moreover, LDA, WC, PBESOL, PBE-GGA were tested for different phases of ZnO, B1(NaCl), B2(CsCl), B3(ZB) and B4(Wurtzite). Hence, the obtained results showed that ZnO Wurtzite is the most stable phase and the approximation GGA is found to be the most accurate approximations to calculate electronic and optical properties. Moreover, a good choice of the calculation parameters improves the results in less time calculations. It was also shown that the band structure, in the most stable phase, presents a direct gap at the Γ point. The deduced gap values, underestimated by the GGA approximation, are corrected by TB-mBJ method to obtain comparable results to experimental work. Then, from the density of states calculations, it was emphasized on the importance of the 3d band effect for ZnO. Finally, for the optical properties, we determined real and imaginary parts of the dielectric function and their average values as well as the compound reflectivity and absorption coefficient. It should be noted that all the investigated structural, electronic and optical properties are in good agreement with those determined experimentally as well as those theoretically reported in literature.

Keywords: ZnO, DFT, Wien2k, physical properties, approximations.

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Theoretical investigation of the electronic and thermodynamic structural properties of the Mn_2ScSi alloy

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Abstract. Among the technologically remarkable compounds, due to their physical properties and their applications, we cite the Heusler alloys for which we devote this work. The aim of this work is to use the first principle calculation method called FP-LAPW, based on the density functional theory (DFT), with the generalized gradient approximation (GGA), to determine the structural stability, the magnetic phase, chemical bonds, electronic and magnetic properties of Mn_2ScSi compounds. The determination of the structural stability of the L_{21} phase of the Cu_2MnAl type. The results obtained show that the compound is ferromagnetic and has a half-metallic character. Based on the Debye quasi-harmonic model implemented in the Gibbs2 code, we determined the thermodynamic properties.This material is a potential candidate for applications in spintronics

Keywords: Heusler alloys; DFT; FP-LAPW; structural stability; thermodynamic properties.

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First Principale calculations of structural,elastic, électronic and magnetic propreties of Ag_2BSm full Heusler alloy comounds using GGA and GGA+U : FP-LMTO calculations

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Abstract. A series of full-Heusler based on rare earth Ag_2BSm are studied by liner muffin-tim orbital FP-LMTO method. Within generalized gradient approximation GGA and GGA+U in the frame of density functional theory DFT. We have studied the structural, elastic, electronic and magnetic properties. We have found that our three compounds are stable in $AlCu_2Mn$ type. The elastic constants at equilibrium are also determined. We have the bulk and shear modulus(G), young's modulus(E), poison's ratio (ν), ratio(B/G) and we have deduced anisotropic parameter (A). From the parameter's behavior, it is inferred that these alloys are elastically stable and ductile in nature. The magnetic moments of both the materials in both cubic phases have been calculated.

Keywords: rare earth, DFT, FP-LMTO, GGA, GGA+U, magnetism.

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Relativistic effects on the structural, electronic and dynamic properties of new hypothetical III-V compounds formed by the group III elements and superheavy element of group V

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Abstract. The quest of superheavy elements (SHEs) belongs to the most fundamentals areas of physical science. Chemical studies of these elements [1-2]are currently the hottest topics chemistry research. Using first-principles calculations within density functional theory, we explore the electronic structure and ground state properties of new hypothetical III-V compounds formed by the group III elements (B, Al, Ga, In, and Tl) and superheavy element of group V: Ununpentium (Uup). Our studies reveal that the proposed hypothetical new III- Uup family divulges surprising features compared with other III-V semiconductors. Furthermore, the calculated partial phonon density of states shows the dynamical stabilities of the predicted ground state phase of all III-Ununpentium compounds.

Keywords: III-Ununpentium; DFT; Fermi surface; partial phonon density of states.

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Theoretical study of the structural electronic properties of half-Heusler KInSn alloy

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Abstract. Recently new combination of atoms from I-III-V are predicted as TI by Vikram et al [1] with 8 valence electron ,these composition don't respect the classical periodic table of Half Heusler such as KInSn, KSnIn, RbInSn ,RbSnIn . this idea is done previously by Zhang et al (2014)[3] but without studying the thermoelectric proprieties. A most of characteristic can be found in half-Heusler with topological behavior [2]. In this work, calculate the structural and the electronic properties of the combination XInSn, XSnIn (X=K) in half Heusler structure which associate to the space group F-34m in order to verify the comportment thermoelectric of these materials. Using the full-potential linearised augmented plane-wave (LAPW) method, implemented in the WIEN2K code and the GGA exchange correlation functional including the spin orbit coupling (SOC) effect. We firstly review the structural and electronic properties then we confirm the topological behavior of theses materials by plotting the band structure curve. We also verify the dynamical stability by phonon dispersion and mechanical stability by calculating the elastic constants. The inversion between the valence band and conduction band confirm the topological character of this material. Finally we calculate the lattice thermal conductivity in order to evaluate the thermoelectric properties for another work.

Keywords: Half Heusler; Topological insulator; band structure; Spin orbit coupling (SOC).

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Investigation of Structural, Elastic, Magnetic and Electronic proprieties for Co_2LuAs Full-Heusler Alloys

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Abstract. A study on the structural, elastic, electronic, magnetic and thermodynamic properties of full-Heusler Co_2LuAs compound by using the first principles calculations and applying the generalized gradient approximation Perdew, Burke and Ernzerhof GGA-PBE for electron exchange and correlation is reported. The GGA+U approximation is used to determine the effect of the Hubbard correction on the magnetic and electronic properties. According to the results obtained for the structural properties, our compound are stable in the regular structure and ferromagnetic states. The elastic properties have shown the conformity of the elastic constants with the stability criteria and the ductile nature of the compound. This mechanical stability is preserved over the interval, 0-50 GPa.The use of the two approximations GGA and GGA+U, showed the effect of the Hubbard correction applied to the atom Co on the variation of it magnetic moment.

Keywords: DFT, Full Heusler, Hubbard potential, magnetic properties.

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The Structural, Electronic, Optical properties of Oxynitride Perovskite $CaTaO_2N$

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Abstract. We carried out ab initio calculations of structural, electronic and optical properties of $CaTaO_2N$ compound in Pnma orthorhombic structure, using the full-potential linearized augmented plane wave method (FP-LAPW), within the framework of density functional theory (DFT). The calculated structural parameters are found to be in good agreement with the experimental results. Moreover, the electronic band structure, total, and partial densities of electron states have studied to explain the origin of bandgaps and the contribution of the nitrogen anion in the valence and the conduction bands. The *Pnma* structure is predicted to be a direct band gap in the direction $\Gamma \rightarrow \Gamma$ with bandgap of 2.32 eV. The optical properties represented by the dielectric functions calculated for $CaTaO_2N$ show that the Pnma structure absorbs the light at a large window in the edge UV-Vis regions.

Keywords: DFT; FP-LAPW, perovskite oxynitrides, band structure, optical properties.

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First principles calculations of structural and optoelectronic properties of XF_3(X= La, Al)

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Abstract. The central idea of our work concerns the theoretical study of the optoelectronic properties of wide band gap materials. This study will be done through a theoretical treatment based on the density functional theory (DFT) [1, 2, 3]. These materials have recently revealed their interest in application fields such as shielding against X-ray radiation. The prediction of structural, mechanical, electronic and optical properties have been performed with the Wien2k and Castep code for the two compounds XF_3 (X= La, Al) in their hexagonal phases. Our structural and optoelectronic properties are in agreement with the available experimental and theoretical data [4, 5, 6].

Keywords: Terre rare, DFT, GGA, tysonite, proprieties mecaniques.

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First-principles calculations of the structural, electronic, mechanical and thermodynamic properties of MAX Phase $Mo_{n+1}GeCn$ (n = 1, 2, and 3) compounds

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Abstract. The MAX phase materials are a new class of carbides and nitrides with the unique combination of metal and ceramic-like properties together which offer new directions to structure modifications for a variety of technological and engineering applications. In this study, we predict the structural, electronic, elastic, mechanical and thermodynamic properties of the $Mo_{n+1}GeCn$ (n = 1, 2, and 3) MAX phase materials via first-principles (density functional theory (DFT)) calculations. The lattice parameters and formation energies are calculated for the simulated MAX phases under consideration. Five independent elastic constants (C11, C12, C13, C33, and C44 = C55) are determined and we have used them to calculate the Young's modulus (E), bulk modulus (B), shear modulus (G), Poisson's ratio (υ) and anisotropy index (A). From our calculations, the predicted electronic band structure and density of states plots show that for the investigated MAX phases, major contribution in the electronic density of states around the Fermi energy originates from the Mo-4d states. The compounds are metals with electrical conductivity arising primarily due to the Mo-4d electrons. Thermal effects on some macroscopic properties (lattice constants, Debye temperature, heat capacity, and thermal expansion coefficient) of $Mo_{n+1}GeCn$ (n = 1, 2, and 3) are investigated by employing the quasi-harmonic Debye model in a temperature range from 0 K to 1000 K and a pressure range from 0 GPa to 40 GPa as well.

Keywords: MAX phase materials, Elastic properties, WIEN2k code, FP-LAPW+ DFT, Thermal properties.

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Ab initio study of structural, electronic and magnetic properties of V-doped ZnS

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Abstract. A theoretical study of the structural, electronic and magnetic properties of various compounds possible transition metal ternaries based on zinc blende ZnS semiconductors is systematically explored using the accurate full-potential linearised augmented plane wave plus local orbitals (FP-L/APW + lo) [1, 2] method that is implemented in WIEN2k [3] computer code. The exchange and correlation (XC) potential is defined by the generalised gradient approximation of Perdew et al. (GGA-PBE) [4]. Half-ferromagnetism metallic is found in V-doped ZnS. Fairly high Curie temperatures would be expected in most of this ferromagnet . This ferromagnetic phase , structurally stable and compatible with this semiconductor, will be useful in spintronics.

Keywords: GGA-PBE, Half-metallic, spintronic.

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The electrodeposition of materials in the synthesis of nanostructures

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Abstract. Materials with particle sizes less than 100 nm are classified as Nanostructured Materials[1]. Due to ultra-small building units and high surface-to-volume ratio, these materials have special properties, such as mechanical, optical, electronic and magnetic properties[2]. The size of the constituent components can be controlled. For example, nanostructured metals and ceramics can improve mechanical properties compared to traditional metals and ceramics[3]. Technological applications of nanostructured materials in the field of energy, such as batteries, Semiconductors in optoelectronic devices such as photodiodes and especially Quantum size effects caused by the spatial confinement of electrons Finite grain delocalization[4]. Several processes make it possible to ensure the deposition of the films in our presentation of the seminar we will talk about the chemical and physical processes and we will explain in particular the processes of electrodeposition.

Keywords: electrodeposition, nanostructures, materials.

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Ab-initio study of the electronic structure of the element Ag

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Abstract. In this work, we have studied the structural, electronic, dynamic and mechanical properties of the element Ag in two different structures; the cubic structure Fm3m, and the hexagonal polytype structure $P6_3mmc$. For this, we have studied an ab-initio method based on the DFT [1], which is the pseudopotentiel method, implemented in the ab initio Quantum espresso code [2]. The electronic study shows the metallic aspect of this material. The analysis of the calculated elastic constants and the phonon dispersion curves reveals that the two studied phases are mechanically and dynamically stable

Keywords: Ag, polytypism, phonon.

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Stabilities and Half-metallic ferromagnets features of new quaternary Heusler alloys RhCoVX (X= Si, Ge and Sn). Ab-initio study

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Abstract.
New quaternary Heusler alloys (QHAs) RhCoVX (X = Si, Ge, and Sn) were investigated for stability and half-metallic ferromagnet features [1]. Three nonequivalent structural arrangements of type I, II, and III structures are considered [2]. Type I is described as the most stable phase for all these compounds in ferromagnetic order compared to non-magnetic order. We also demonstrate the thermodynamic, dynamic, and mechanical stability of RhCoVX (X = Si, Ge, and Sn) by computing the cohesive energies [3], formation energies, phonon dispersion curves, and elastic constants. Using GGA-mBJ and LDA-mBJ calculations show that RhCoVX (X = Si, Ge, and Sn) are half-metallic ferromagnets (HMFs), with indirect band gap through the altered Becke-Johnson (mBJ), in the two approach's LDA-mBJ and GGA-mBJ: 1.03 eV (0.922 eV) for RhCoVSi, 0.956 eV (0.856 eV) for RhCoVGe and 0.706 eV (0.662 eV) for RhCoVSn. Furthermore, the electrons at the Fermi level (EF) were fully spin-polarized. The total magnetic moment in these three compounds was found as an integer value of $3.00\mu B$ per formula, which complies with the Slater-Pauling rule $M_t = Z_t - 24$. According to the given results, these compounds are promising materials for spintronic applications. All calculations used the density functional theory (DFT) based on the full-potential linearized augmented plane wave (FP-LAPW) method implemented in the WIEN2K code.

Keywords: Quaternary Heusler, First principle calculations, Half-metallic, Spintronic.

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First-principles calculations of structural, elastic, dynamic, electronic, and magnetic properties of Co_2FeSi full-Heusler alloy

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Abstract.
First-principles calculations of the electronic structure, magnetism and dynamic stability of transition-metal-based full-Heusler alloy with the chemical formula X_2YZ [1, 2] is presented and discussed with a goal of identifying compounds of interest for spintronics. All calculations were performed using first-principles full-potential linearized augmented plane-waves method based on density functional theory (DFT). The current work has been carried out within the Perdew-Burke-Ernzerhof (PBE) under generalized gradient approximation (GGA) for the exchange-correlation energy and potential. In the first part as far as we know, it is the first time to research the dynamical stability of Co_2FeSi full-Heusler alloys in theory. From the total energy calculation using two possible structural Cu_2MnAl and Hg_2CuTi phases, it is found that Co_2FeSi full-Heusler alloy is stable and half-metallic ferromagnet in the ferromagnetic (FM) Cu_2MnAl phase. The spin-polarized density of states of the Co_2FeSi full-Heusler alloys shows that the majority spin channel has metallic nature and the minority spin channel has a gap, resulting in a stable half-metallic ferromagnetic (HMF) behavior with magnetic moment of 5 μB per formula unit. Presence of HMF in Co_2FeSi full-Heusler alloy makes this alloy promising material for spintronic applications.

Keywords: Density functional theory, Full-Heusler alloy, Ferromagnet, Phonon, Phase stability.

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The investigation on structural, electronic, magnetic and thermodynamic properties of half-metallic materials via first-principles calculations based on density functional theory

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Abstract.

This paper reports the structural, electronic, magnetic, and thermodynamic properties of Ti-doped ordered rock-salt CaS, CaSe semiconductors at a fixed concentration (x = 0, 25). All systematic calculations are performed using the full-potential linearized augmented plane wave method (FP-LAPW) with a density functional theory (DFT) implemented in WIEN2K package [1, 2]. It is verified that all the investigated compounds are in a stable ferromagnetic phase (FM) in comparison to the non-magnetic phase (NM). The electronic properties (band structure, electronic density of state) have a half-metallic ferromagnetic (HMF) behavior with 100% spin polarization at the Fermi level (E_F) for $Ca_{0.75}Ti_{0.25}S$, $Ca_{0.75}Ti_{0.25}Se$. This characteristic results from the metallic and semiconducting natures of majority-spin and minority-spin channels. In addition, the analysis of the magnetic properties of $Ca_{0.75}Ti_{0.25}M$ (M=S, Se) alloys indicate that the value of the total magnetic moment is equal to $2\mu B$ per Ti atom. Furthermore, the thermodynamic properties are studied and investigated using the quasi-harmonic model. In all compounds, to evaluate the effects of the exchange splitting process, the conduction and valence band –edge spin splitting $\Delta E_c(eV)$ and $\Delta E_v(eV)$ and the exchange constants $N_{0\alpha}$ and $N_{0\beta}$ are predicted. Finally, our prevision results confirmed that $Ca_{0.75}Ti_{0.25}M$ (M=S, Se) could be considered as a promising candidate material for spintronics applications.

Keywords: Ti-doped Ca chalcogenides, Half-metallic ferromagnetic, Electronic structure, Magnetic Properties, Thermodynamic properties, Ab initio Calculations.

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The theoretical prediction of $CuMg_2AlS_4$ quaternary chalcogenide

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Abstract.
We used FP-LAPW method [1] , as implemented in WIEN2k code [2], to investigate the structural, and electronic properties of $CuMg_2AlS_4$ compound. GGA with the Perdew-Burke-Ernzerhof (PBE) [3] correlation energy functional was used to calculate the exchange-correlation potential. The obtained value of K-points and R.Kmax, ensuring the convergence of the total energy of the system, are found to be 600 and 8, respectively. RMTs are taken to be 2.16, 1.8, 1.82, 1.84 for Cu, Mg ,Al and S, respectively. The cut-off energy was chosen to be -6 *Ry*, while the energy and charge convergences were chosen to be 10-6 *Ry* and 10-5 e, respectively. Our compound $CuMg_2AlS_4$ crystallize in three structures: First, in tetragonal structure ($a = b \neq c$ and $\alpha = \beta = \gamma = 90$), with Kesterite phase (KS)(space group I-4; N79), and stannite phase pace (ST) (space group $I-42m$; N 121). Second, in orthorhombic structure ($a \neq b \neq c$ and $\alpha = \beta = \gamma = 90$), with wurtzite-stannite phase (WS) (space group $Pmn21$; N31) [4]. Finaly, in monoclinic structure ($a \neq b \neq c$ and $\alpha = \beta = 90$, $\gamma \neq 90$) (space group PC; N7). The change in total energy with respect to the volume per formula unit for our compound, indicates that the PC phase is the most stable one. According to band structure our compound is semiconductor with direct band gap of 3.05 eV.

Keywords: Gap, Semiconductor, Electronic properties.

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Enhancement of the magneto-electronic properties by GGA and TB-mBJ approaches for $KBeO_3$ perovskite oxide

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Abstract.
We investigate the structural, elastic, electronic and magnetic properties of $KBeO_3$ using first-principle calculations, based on the formalism of the density functional theory (DFT) [1] and the method of Full potential augmented and linearized plane waves (FP-LAPW) [2] implemented in the Wien2k code. The exchange and correlation effects were treated by the following two approximations: generalized gradient approximation (GGA) [3] and Tran-Blaha modified beck Johnson (TB-mBJ) [4] potentials. After analyzing the obtained structural parameters, the results revealed that $KBeO_3$ compound is most stable in its ferromagnetic configuration. The formation energy value showed that this compound can be experimentally synthesized.Furthermore,the calculated band structures, and density of states (DOSs) indicate the half-metallic behavior of $KBeO_3$. We found also that the total magnetic moment is an integer value of 3 μB which confirms the half-metallic character. The magnetic moment especially issues from the spin-polarization of p electrons of O atoms. The Curie temperature is estimated to be $639K$ within the mean field approximation (MFA) [5].

Keywords: FP-LAPW, Perovskite, Half-metallicity, Ferromagnetic.

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Comparative study of optoelectronics, mechanical, dynamic properties of GaAs, GaP, and GaAsP compounds

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Abstract.
Due to the increasing demand of high performance optoelectronic and photonic devices, comparative study of GaAs, GaP and GaAsP compounds was carried out to study the optoelectronic, mechanical, dynamic properties in response to the changed polytypes 3C, 6H, 4H, 2H by applying the state-of-the-art first-principles pseudopotential calculations as implemented in the ab initio Quantum espresso code [1]. Optoelectronics Results show that GaAs emits infrared wavelength in the four polytypes. However, in GaP, the green emission turns to green-yellow from 6H to 4H polytypes, and to yellow-orange in the 2H. Additionally, GaAsP hexagonal polytypes emits visible red wavelengths. We show that all the studied materials are mechanically and dynamically stable in the cubic and wurtzite 2H, 4H and 6H bulk form.

Keywords: Gallium phosphide, GaAsP, Wavelength, Polytypes, Phonon, Quantum espresso.

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First-principles study of structural, electronic, magnetic properties and elastic anisotropy of $Sr_{1-x}TM_xS$ (TM = Fe, Co)

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Abstract.
We have performed a first-principles study to investigate the electronic structure,the magnetic, elastic and mechanical properties strontium sulfide SrS semiconductor doped with transition metal impurities Fe and Coi.e. $Sr_{1-x}TM_xS$ (TM = Fe, Co) at concentration x = 0.25 using the full-potential linearized augmented plane wave (FP-LAPW) approach to the density functional theory (DFT). Total energy calculation allowed us to determine the ground-state parameters, namely the lattice constant, the bulk modulus ant its first pressure derivative.The electronic properties are calculated using both the generalized gradient approximation proposed by Wu and Cohen (GGA+WC) and the Tran Blaha modified Becke-Jonhnson (GGA-TBmBJ) for the exchange and correlation potential. The $Sr_{0.75}Fe_{0.25}S$ is found to be half-metallic ferromagnet with a total magnetic moment of 4 μB while $Sr_{0.75}Co_{0.25}S$ is a metallic ferromagnetic compound and its total magnetic moment is 2.957 μB. We also report results on elastic constants and mechanical properties of these compounds. The objective is to seek new ferromagnetic materials for an application in the new emerging field of spintronics and the studied compounds are suitable candidate for such application [1, 2].

Keywords: First-principles calculation, Spintronics, Electronic structure, Half-metallic ferromagnets, Elastic Anisotropy.

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First principles calculations of electronic and magnetic properties of Perovskite $NdGdO_3$: a theoretical study

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Abstract. The electronic and magnetic properties of $NdGdO_3$ perovskite have been studied using the full-potential linearized augmented plane wave method (FP-LAPW) based on the density functional theory (DFT) implemented in Wien2K code [1]. The exchange and correlation potential were treated within the generalized gradient approximation (GGA)[2].The results reveal that $NdGdO_3$ exhibits half-metallic behavior with an integer magnetic moment of 10 μB per cell. Our result show that $NdGdO_3$ could provide a new type of material, named half-metallic for future spintronic devices.

Keywords: First principles calculations, Perovskite, $NdGdO_3$, Half metallic, Magnetic properties, Electronic properties, Band structure, Spintronic.

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Ab-initio study of electronic structure and magnetism in the rare-earth-based half-Heusler GdPdBi alloy

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Abstract.
Very recently, based on first-principle calculations, a topological insulating state has been predicted in half-Heusler phases containing a rare earth element [1, 2]. Some half-Heusler alloys of the XYZ type (X = rare earth element) have been shown to exhibit band inversion similar to that found in the binary compound HgTe. In this work, we focused on a novel rare earth element-based ternary half-Heusler alloy as an f-type potential magnetic system. To this end, we performed a first-principle calculation based on the density functional theory (DFT) with spin polarization to explore the structural, elastic, thermodynamic, electronic and magnetic properties of the half-Heusler GdPdBi ternary alloy in different phases α, β and γ. To our knowledge, there is no experimental study on this type of half-Heusler alloy. We have found that this alloy is a semi-metal in both spin polarization directions, with potential applications in spintronic devices.

Keywords: DFT, Ferromagnetism, Phonon, Heusler, Rare earth element.

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Investigation of structural, electronic, magnetic and half-metallic properties in ternary Half-Heusler alloy FeVGe : FP-LAPW calculations

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Abstract.
First-principles calculations based on density functional theory (DFT) using the WIEN2k code [1] with the self-consistent full potential linearized augmented plane wave (FP-LAPW) method [2] are used to calculate the structural, electronic, elastic, magnetic and half metallic properties of the FeVGe Half-Heusler alloy. Firstly we have considered both cubic and hexagonal structures ($C1_b$-type and ZrBeSi-type respectively), and the effect of spin-polarization has been studied, in order to find the most stable structure and the ground state energy, we found that the $C1_b$-type structure in magnetic phase makes the ground state at equilibrium lattice constant a= 5.587Å. Then we show that our compound exhibit a half-metallic (HM) character and have a magnetic moment of 1.00 μB per formula unit. This latter statement is coherent with the generalized Slater-Pauling rule (SP)[3, 4]. From the band structure and density of states calculations, we explain the formation of the indirect energy band gap in the spin-majority channel. The mechanical stabilities of the FeVGe compound have been analyzed according to the elastic constants; it is obvious that, from our values taken from the Mehl model satisfy the stability criteria of a cubic material, indicating that the FeVGe alloy is mechanically stable.

Keywords: DFT, Half-metallic ferromagnetism, Electronic structures, Half-Heusler alloys.

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Magnetic properties of $GaN/(MnN)_n/AlN/(CrN)_n$, $GaN/(MnN)_n/AlN/(VN)_n$, $GaN/(CrN)_n/AlN/(VN)_n$ superlattices (n= 1, 2)

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Abstract.
Using density functional theory, we have studied the electronic and magnetic properties of $GaN/(MnN)_n/AlN/(CrN)_n$, $GaN/(MnN)_n/AlN/((VN)_n$, $GaN/(CrN)_n/AlN/(VN)_n$ superlattices (n= 1, 2). The calculations were performed in the framework of density functional theory (DFT). We have employed the full potential linearized augmented plane wave (FPLAPW) method as implemented in the WIEN2k code [1]. We demonstrate the possibility to obtain half-metallic ferromagnets in GaN/MnN/AlN/CrN, GaN/(MnN/AlN/VN, GaN/CrN/AlN/VN with a total magnetic moment close to 14μB , 12 μB, and 10 μB for GaN/MnN/AlN/CrN, GaN/(MnN/AlN/VN), GaN/CrN/AlN/VN respectively . The ferromagnetism can be explained by the contribution of Mn and Cr and V atoms and the interstitial region [2, 3].

Keywords: Magnetic properties, Superlattice, Wien2K, DFT, FP-LAPW.

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First principles calculations of electronic and magnetic properties of Perovskite $NdGdO_3$: a theoretical study

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Abstract. The electronic and magnetic properties of $NdGdO_3$ perovskite have been studied using the full-potential linearized augmented plane wave method (FP-LAPW) based on the density functional theory (DFT) implemented in Wien2K code [1]. The exchange and correlation potential were treated within the generalized gradient approximation (GGA)[2].The results reveal that $NdGdO_3$ exhibits half-metallic behavior with an integer magnetic moment of 10 μB per cell. Our result show that $NdGdO_3$ could provide a new type of material, named half-metallic for future spintronic devices.

Keywords: First principles calculations, Perovskite, $NdGdO_3$, Half metallic, Magnetic properties, Electronic properties, Band structure, Spintronic.

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Ab-initio investigation of structural, electronic and elastic properties of Ru_2CuGe full-Heusler alloy

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Abstract.
We investigate the structural, electronic and elastic properties of the Heusler compound Ru_2CuGe performed with the ab-initio code WIEN2k [1], using the full-potential linear-augmented plane-wave method (FP-LAPW) [2] in the framework of the density functional theory (DFT) [3], using the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE). The analysis of structural properties shows that the cubic structure $L2_1$ (SG N 225) makes the ground state of Ru_2CuGe full-Heusler alloy. Our calculation was carried out in both ferromagnetic (FM) and non-magnetic (NM) phases, it was found to be more stable in the non-magnetic phase at equilibrium lattice constant $a = 5.99$Å, in addition, the electronic properties revealed the metallic character of Ru_2CuGe full-Heusler alloy. Finally, the study of the elastic properties of the Ru_2CuGe Full-Heusler alloy is the indispensable tool that proves the mechanical stability

Keywords: DFT, GGA, Heusler alloys, FP-LAPW.

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First-principles study of the half-metallic behavior in the full-Heusler $Co_2MnTi_{1-x}Al_x$ alloy

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Abstract.
Ab-initio calculation method was used to study the dynamical, thermal, mechanical, magnetic and electronic properties of the full-Heusler alloy Co_2MnV using the (FP-LAPW) method. We have studied these properties in the following two structures cubic $L2_1$ ($Fm3m$) and the inverse phase $C1_b$ ($F\bar{4}3m$) phases [1, 4] in the configuration ferromagnetic. The most interesting aspects of these alloys are the half-metallic, the stability thermodynamic and mechanic. The results show that the dynamical, and mechanical properties of the Co_2MnV is stable in the $L2_1$ structure, and we found the Co_2MnV is half-metallic ferromagnet then these results are good agreement with experimental and theoretical have been reported Thus, these results show that alloys are very good in the spintronic devices.

Keywords: DFT, Phase stability, Full-Heusler alloys, Ferromagnetic.

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Theoretical investigation of structural, electronic and magnetic properties of Ti-based full-Heusler alloy

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Abstract.
In this paper, we performed an ab initio calculation of the different properties of the Ti-based full-Heusler alloy [1, 2] which is reported for the first time using the WIEN2k implementation of the full potential linearized augmented plane wave (FP-LAPW) scheme. In order to study this alloy for magneto-electronic applications we used the generalized gradient approximation (GGA) for its mechanical properties and the mBJ-GGA to better investigate the electronic properties. Our results show that the Ti_2VPb full-Heusler alloy exhibits half-metallicity at its equilibrium lattice constant 6.548 Å, but a metallic character would occur with an expansion of its lattice parameter to 6.85 Å.

Keywords: Density functional theory, FP-LAPW, Full-Heusler alloy, Ferromagnetism.

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Ab-initio study of structural, elastic, electronic, and magnetic properties of Mn_2FeAl full-Heusler alloy

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Abstract.
Spin-polarized density functional theory studies were performed for the structural, dynamic, thermodynamic, electronic, and magnetic properties of full-Heusler Mn_2FeAl alloy. The generalized gradient approximation for the exchange-correlation energy and potential was used. The variation of the energy as a function of the volume showed that Mn_2FeAl alloy is more stable in the $L2_1$-type and XA-type ferrimagnetic structures. Considering the phonon dynamics of full-Heusler Mn_2FeAl alloy, we observed that this alloy is dynamically stable in both the $L2_1$-type and XA-type structures. The full-Heusler Mn_2FeAl alloy was observed to be metallic in the ferrimagnetic $L2_1$ and XA-type structures with magnetic moments of $1.41\mu B$ and $2.90\,\mu B$ per formula unit, respectively. The spin-polarized density of states and band structures showed that the full-Heusler Mn_2FeAl alloy in the $L2_1$ and XA-type structures is metallic in both the minority and majority spin channels. This confirms the metallic nature of the Mn_2FeAl alloy in the $L2_1$ and XA-type structures, which makes this alloy promising material for spintronic applications [1–4].

Keywords: Density functional theory, Phase stability, Phonon, Heusler alloys, Ferrimagnetic.

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Oxygen-functionalized W_2C MXeneas anode material for Na-ion battery: A first-principles study

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Abstract.
At present, the largest and most wide spread energy storage technology from electric vehicles to the various electronic devices available on the market consists exclusively of secondary batteries. In particular, Lithium-ion-based rechargeable batteries (LIBs) [1–3]. However, scarcity of lithium and high processing costs, implies that it cannot single-handedly meet the increasing demand of the future and it is important to find alternative batteries for LIBs. Sodium (Na), an alkali metal has similar chemical characteristics to lithium (Li), and more abundance on earth. In this work, we have studied oxygen terminated $2D$ tungsten carbide (W_2CO_2) as anode for SIBs by using first-principles calculations. In order to verify the dynamical stability of (W_2CO_2) we have calculate the molecule dynamic and phonon properties,the obtained results confirm that W2CO2 is dynamically stable upon $300K$. The calculated adoption energy of one Na atom on a $3 \times 3 \times 1$ surface is -3.066 eV. (W_2CO_2) monolayer exhibits relatively low diffusion barrier (0.18 eV). Furthermore, the maximum theoretical specific capacity of (W_2CO_2) monolayer as Na-ion batteries is $260mAh/g$ for double side adsorption.

Keywords: (W_2CO_2), Anode materials, Na-ion battery, First-principles calculations.

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Investigating new stable phases for the ternary alloy II-VI of $Sr_xCa_{1-x}O$: DFT study

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Abstract.
The structural stability, electronic, and mechanical properties of newly identified structures for the alloy $Sr_xCa_{1-x}O$ are investigated through the density functional theory (DFT) [1]. According to the dynamic, thermodynamic, and elastic constants, the title compound is stable. The mechanical properties show a decrease of the elastic moduli by increasing the composition x of Strontium, and the system remains brittle. The results show that the alloy becomes more resistant to thermal shock in Strontium rich environment, and it can be easily distorted. Moreover, the energies bandgaps are around 5 eV and are globally direct at Γ point which indicates that $Sr_xCa_{1-x}O$ is a potential candidate for optoelectronic devices in UV-region, and it is recommended to be used as a protective layer

Keywords: $Sr_xCa_{1-x}O$, ternary alloy, DFT, phonon, electronic properties, mechanical properties.

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First-principles study of the half-metallic behavior in the full-Heusler $Co_2MnTi_{1-x}Al_x$ alloy

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Abstract.
Ab-initio calculation method was used to study the dynamical, thermal, magnetic and electronic properties of the full-Heusler alloys Co2MnTi1-xAlx (x= 0, 0.25, 0.50, 0.75, 1) using the FP-LAPW method. We have studied these properties in the following two structures: cubic L_{21} (and the inverse phase C1b phases in the ferromagnetic configuration. The most interesting aspects of these alloys are the half-metallic and the thermodynamic stability. The results show that the dynamical properties of the full-Heusler alloys $Co_2MnTi_{1-x}Al_x$ (x= 0, 0.25, 0.50, 0.75, 1) are stable in the L_{21} structure, and we found that the $Co_2MnTi_{1-x}Al_x$ (x= 0.25, 1) is half-metallic ferromagnet. These results are in quite good agreement with experimental and theoretical results which have been reported so far. Therefore, these results show that the proposed alloys are good candidates for spintronic devices applications.

Keywords: DFT; Phase stability; full-Heusler alloys; Ferromagnetic.

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Electronic, elastic and lattice dynamical properties of the half-heusler alloys KMgX (X= P, As).

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Abstract.
Half-Heusler alloys are excellent materials for diverse applications such as opto-electronics, electrical, and thermoelectric applications [1]. The electronic properties of the Zinc Blende KMgP and KMgAs are studied using the generalized gradient approximation by the Tran Blaha modifed Becke Johnson's potential (mBJ) [2]. These compounds exhibit a direct band gap [3]. As the dynamical and elastic properties of the half-Heusler KMgP and KMgAs are calculated by the plane wave pseudo-potential (PW) methods, within the generalized gradient approximation (GGA). We have obtained the elastic constants and the frequencies of selected phonons modes for these half-Heusler compounds.

Keywords: Half-Heusler, KMgP, KMgAs, mBJ-GGA, Phonons.

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8 Nanostructures and Nanomaterials (NSN)

8.1 Plenary Session

8.2 Oral session

8.2.1 *Tin and indium promoted silicon nanowires growth via plasma assisted vapor-liquid-solid process*

Tin and indium promoted silicon nanowires growth via plasma assisted vapor-liquid-solid process

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Abstract.
Silicon nanowires (SiNWs) have received considerable attention as base materials for third-generation photovoltaic devices because they lend themselves to large- scale production with enhanced light trapping and increased overall performance. As the properties of tin and indium, nanoparticles govern the properties of the SiNWs. In the present study, silicon nanowires have been grown on p-type boron-doped (100) oriented monocrystalline silicon wafers (c-Si), hydrogenated amorphous silicon (a-Si:H/c-Si) and hydrogenated amorphous silicon carbide (a-SiC:H/c-Si) and hydrogenated silicon germanium (a-SiGe:H/c-Si) substrates by Tin and Indium catalysts coating with a thickness of 1 *nm* via plasma-enhanced chemical vapor deposition (PECVD). The surface characteristics of the prepared Si NWs were performed with field emission scanning electron microscopy (FE-SEM), X-ray diffraction (XRD) and Raman analysis. The FE- SEM images reveal that the prepared SiNWs were tapered and clearly show a change in the morphology and the density with the substrates and the catalyst type. The SiNWs grown on the different substrates had quite different structural characteristics. The presence of strong Si diffraction peaks in all these patterns indicates the as-grown SiNWs are highly crystalline in structure. These results are confirmed by the Raman analysis. The results presented in this work can be used to aid selection of appropriate substrates and metal catalyst for SiNW growth, depending on specific applications [1–3].

Keywords: Silicon nanowires, Tin, Indium, plasma-assisted VLS.

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Elaboration and Characterization of a New PVA-CMC/Fe_2O_3 Semiconductor Composite Biomateria

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Abstract.
Ferrogel is a smart material that combines the elastic properties of hydrogel and the magnetic charging behavior of magnetic materials. In this work the preparation of hybrid hydrogels of poly (vinyl alcohol) PVA and carboxymethyl cellulose CMC under different conditions was proposed. PVA/CMC/Fe_2O_3 ferrogels were made using physical crosslinking by the freeze-thaw method. PVA/CMC hydrogels and PVA/CMC/Fe_2O_3 biocomposites were characterized by FTIR, UV-Visible and thermal ATG and DSC spectroscopic analyses.Our materials were then tested by a study of the kinetics of the swelling rate, the biodegradation test and the antibacterial activity. The effect of the addition of the Fe2O3 filler on the resistance of the material to deformation and the optical properties was studied. Applying manual compression to our PVA/CMC hydrogels and PVA/CMC/Fe_2O_3 biocomposites results in reversible deformation after the applied force is removed. The extensibility of the PVA50/CMC50 composite hydrogel is improved by about 40% by adding 1% Fe_2O_3. Unlike for the PVA80/CMC20 composite hydrogel, a decrease in extensibility of approximately 46 % is observed by the addition of a small amount of Fe_2O_3 of 0.5%. The addition of iron oxide improved the strength and crystallinity of the hydrogel. The type of additive nanoparticles or Fe2O3nanofillers in the tested hydrogels shows an interesting role in modifying the bandgap energy of the tested composite hydrogels. The energy of the allowed direct or indirect band gaps Eg decreases in the PVA/CMC hydrogel matrix by increasing the conjugation between the unsaturated bonds of PVA/CMC and the nanoparticles of $\alpha - Fe_2O_3$ [1].

Keywords: Hydrogel, Ferrogel, CMC-PVA, biocomposites, Extensibility, Eg optical gap, Semiconductor.

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Porous Carbon as a low-cost Pt-free counter electrode for dye-sensitized solar cell

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Abstract. The counter electrode (CE) is an important part of dye-sensitized solar cells (DSSCs). Platinum Pt CEs show high-performance in DSSCs using iodide-based electrolytes. However, the high cost and dearth of resources of Pt restricts their large-scale application in DSSCs and the development of Pt-free CE is expected. Carbon can be replaced Pt because of their good catalytic properties and low cost [1]. In this research, porous carbon film is prepared as the Pt-free CE and porous TiO_2 film as photo-anode for DSSC; both films were deposited on the transparent conducting oxide substrates by doctor Blade technique. The morphological, structural and electrical properties of these films were studied using (SEM,XRD and impedance spectroscopy). The DSSC was fabricated from these films using an electrolyte based on iodide and the photo-anode based TiO_2, sensitized with the organic dye coumarin ($C343$). The current–voltage measurements reveal that the DSSC based on the porous carbon CE exhibit (VOC= 0.450 V, J_{SC}= 1.75 mA/cm^2, FF = 0.51 and PCE=0.41 %) which are lower than DSSC based on platinum (Pt) CE [2]. The results show that low-cost porous carbon CE is a promising alternative to Pt CE in DSSCs [1–3].

Keywords: Dye-sensitized solar cells, Carbon, counter electrode, Platinum, TiO_2, Porous..

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Nano-reinforced composite structures on elastic foundation: Free vibration analysis

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Abstract. The present study aims to investigate the free vibration of functionally graded single walled carbon nanotube reinforced PMPV polymeric matrix composite sandwich plates considering the first order shear deformation plate theory. Two types of simply supported composite sandwich plates with face sheet reinforced and homogeneous core and with homogeneous face sheet and reinforced core are considered. The face sheet layers or the core layers are reinforced by single walled uniaxially aligned carbon nanotubes in a polymeric matrix with two types of carbon nanotubes distribution across the plate thickness, namely, the uniform distribution and the functionally graded distribution. The material properties of PMPV polymer composite plates reinforced by carbon nanotubes are assumed by employing the rule of mixture. The sandwich plates resting on the Pasternak elastic foundation, including a shear layer and Winkler spring, are considered.The mathematical model of the composite sandwich plate has been derived and the equations of the motion are obtained using Hamilton's principle.The closed form solution of simply supported rectangular sandwich plates has been obtained by using Navier's method.Then, the influence of various parameters of composite sandwich plate such as type of reinforcement, carbon nanotubes volume fraction,aspect ratio, foundation parameters and length to thickness ratio on the free vibration analysis of carbon nanotube reinforced PMPV polymer composite sandwich plates are studied.Results suggest that the functionally graded face sheet reinforced composite sandwich plate has a high resistance compared to the other types of reinforcement [1–3].

Keywords: Free vibration, Carbon Nanotube, Nano-reinforced, Composite, Sandwich Plate, Elastic foundation.

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The effect of carbon nanotube on microelectronics

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Abstract. The laws of physics indicate that the 10 nanometers (for the grid length of the transistor) mark the death stop of the current microelectronics with CMOS transistors. And until now, carbon nanotubes have been considered as a major challenger, without it having been demonstrated that transistors developed in this technology with a grid length of less than 10 nanometers can be achieved. This is now done and the promises go beyond the researchers' expectations since the simulation models developed were pessimistic in relation to the results obtained [1, 2]. The technology consists in developing carbon nanotube transistors on a substrate made with ultra-thin insulation. Carbon nanotubes have the particularity of having a very high electronic mobility. It is this high electron mobility that makes it possible to obtain fast systems able to lay the foundations of future ultra fast processors [3]. Finding an alternative to the current microelectronics is vital. This is because it relies on the reduction of transistor sizes in order to reduce the cost of chips (more chips on the same silicon wafer) and at the same time increase their performance (faster processors) while reducing power consumption. The nanotube transistor consumes much less than any other transistor of the same size. It is also much more efficient thanks to a higher output impedance transconductance product. This makes it easier to amplify the signal [4]. In this paper we will demonstrate the limitations of microelectronics technology as well as the interest of carbon nanotubes in overcoming the problems of miniaturization and improving microelectronics technology.

Keywords: Carbon nanotube, microelectronics, carbon nanotube transistor, interconnect.

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Electrical properties and affinity towards hydrogen to the nanoparticuls Cu^0-loaded SBA-15@ZnO

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Abstract. A nanomaterial was prepared using SBA-15 silica as a seed to grow a zinc oxide (ZnO) shell, followed by a dispersion of uncharged copper nanoparticles (Cu^0) [1,2]. The resulting Cu/SBA-15@ZnO nanostructures show a higher specific surface area and many small pores compared to the SBA silica starting material. The dispersion of the copper nanoparticles (Cu^0NPs) leads to a densification of the host matrix and a significant degradation of the hydrophilicity. This is a further explanation for the significant increase in surface area and decrease in average pore size. The incorporation of ZnO and Cu^0NPs was shown to shift the UV-Vis absorption band towards longer wavelengths, decrease the optical band gap energy and improve the conduction properties. Compared to Zn^0, Cu^0NPs resulted in a strong increase in conductivity, which increased at higher frequencies. Cu/SBA-15@ZnO also showed a higher affinity for hydrogen compared to SBA-15/ZnO and SBA-15 under ambient conditions [3]. These extraordinary properties combined with remarkable thermal stability could open up promising prospects for Cu^0/SBA-15/ZnO as sensors, electrode materials, electrocatalysts and/or hydrogen capture matrices

Keywords: SBA-15, copper nanoparticle, zinc oxide, sensor, conductance.

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Elaboration and Characterization of a New PVA-CMC/Fe_2O_3 Semiconductor Composite Biomaterial

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Abstract. Ferrogel is a smart material that combines the elastic properties of hydrogel and the magnetic charging behavior of magnetic materials. In this work the preparation of hybrid hydrogels of poly (vinyl alcohol) PVA and carboxymethyl cellulose CMC under different conditions was proposed. PVA/CMC/Fe_2O_3 ferrogels were made using physical crosslinking by the freeze-thaw method. PVA/CMC hydrogels and PVA/CMC/Fe_2O_3 biocomposites were characterized by FTIR, UV-Visible and thermal ATG and DSC spectroscopic analyses. Our materials were then tested by a study of the kinetics of the swelling rate, the biodegradation test and the antibacterial activity. The effect of the addition of the Fe_2O_3 filler on the resistance of the material to deformation and the optical properties was studied. Applying manual compression to our PVA/CMC hydrogels and PVA/CMC/Fe_2O_3 biocomposites results in reversible deformation after the applied force is removed. The extensibility of the PVA50/CMC50 composite hydrogel is improved by about 40% by adding 1% Fe_2O_3. Unlike for the PVA80/CMC20 composite hydrogel, a decrease in extensibility of approximately 46% is observed by the addition of a small amount of Fe_2O_3 of 0.5%. The addition of iron oxide improved the strength and crystallinity of the hydrogel. The type of additive nanoparticles or Fe_2O_3 nanofillers in the tested hydrogels shows an interesting role in modifying the bandgap energy of the tested composite hydrogels. The energy of the allowed direct or indirect band gaps Eg decreases in the PVA/CMC hydrogel matrix by increasing the conjugation between the unsaturated bonds of PVA/CMC and the nanoparticles of α-Fe_2O_3. Nanocomposite hydrogels become more semiconductive in nature with increasing iron oxide nanoparticle content. PVA-CMC hydrogel demonstrates high water absorption capacity, necessary flexibility, biodegradability, biocompatibility and elasticity with significant thermal properties at high PVA content.

Keywords: Hydrogel, ferrogel, CMC-PVA, biocomposites, extensibility, Eg optical gap, semiconductor.

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8.3 Poster

8.3.1 *Synthesis and Characterization of CMC-g-PMMA Graft Copolymers and CMC-g-PMMA/TiO_2 Nanocomposites; Fe_2O_3*

Synthesis and Characterization of CMC-g-PMMA Graft Copolymers and CMC-g-PMMA/TiO_2 Nanocomposites; Fe_2O_3

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Abstract. CMC-g-PMMA graft copolymers based on a biopolymer of the polysaccharide family carboxymethylcellulose CMC and a synthetic polymer methyl methacrylate PMMA were synthesized in a homogeneous aqueous medium by radical polymerization by adding persulphate of ammonium as initiator. To improve the properties and diversify the applications of our products, nanocomposites have been developed based on these copolymers and metal oxides as fillers (CMC-g-PMMA/TiO_2 and CMC-g-PMMA/Fe_2O_3). The graft copolymers and their nanocomposites were characterized by spectroscopic FTIR, NMR1H, UV and swelling test analyzes and measurement of electrical conductivity. The results of the analyzes showed that the CMC-g-PMMA copolymer is obtained successfully. The incorporation of TiO_2 and Fe_2O_3 nanofillers increased the absorbance and electrical conductivity of our graft copolymers

Keywords: carboxymethylcellulose CMC, graft copolymers, nanocomposite, poly(méthacrylate de méthyl) PMMA, UV-visible.

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The stability of 1D nanostructured materials

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Abstract. Structural elements such as beams, plates, and nanoscale membranes, are often employed in advanced technological devices such as sensors, actuators, transistors, and resonators in nanoelectromechanical systems (NEMSs). In this article, various higher-order shear deformation theories are developed for bending behaviors of nanowires 1D including surface stress effects [1]. The most important assumption used in different proposed beam theories is that the deflection consists of bending and shear components, Gurtin-Murdoch [2] proposed a theoretical formulation to consider this surface stress impact. Numerical results are illustrated to prove the difference between the response of the nanowires predicted by the classical and non-classical solutions which depends on the magnitudes of the surface elastic constants.

Keywords: Surface effects, Nanowires, Gurtin-Murdoch.

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Fe(0)-SBA-15 nanoparticles as potential hydrogen adsorbents and sensors

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Abstract. The iron-SBA-15 material was synthesized via the incorporation of Fe0 nanoparticles (Fe(0)-Nps) into the mesoporous channels. Electron microscopy and X-ray diffraction showed that the dispersion of these fine iron nanoparticles occurs mainly within the channels of SBA-15 [1], producing a slight compaction of the structure. This was accompanied by a significant improvement in both hydrogen affinity and electrical conductivity, as evidenced by hydrogen adsorption tests and impedance measurements [2]. Programmed thermal desorption measurements of CO2 revealed an attenuation of the acid character of the solid surface. This was explained in terms of the strong interaction of iron with lattice oxygen atoms which reduces the polarity of the SiO-H bond. The presence of Fe(0)-Nps combined with the large pore size of SBA-15 seem to contribute to a synergistic enhancement of the electrical conductivity [3]. The reported results open new perspectives for SBA-15 as potential adsorbents for hydrogen storage and carriers for hydrogen sensors. The use of iron instead of noble metals to design such materials is a novelty, as such applications of iron-filled silica were not considered until now due to the high reactivity of iron towards air and water. The development of such nanotechnologies should solve this problem

Keywords: SBA, Nanoparticle, Iron, Sensor, Storage.

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The electrodeposition of materials in the synthesis of nanostructures

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Abstract. Materials with particle sizes less than 100 *nm* are classified as Nanostructured Materials [1]. Due to ultra-small building units and high surface-to-volume ratio, these materials have special properties, such as mechanical, optical, electronic and magnetic properties [2]. The size of the constituent components can be controlled. For example, nanostructured metals and ceramics can improve mechanical properties compared to traditional metals and ceramics [3]. Technological applications of nanostructured materials in the field of energy, such as batteries, Semiconductors in optoelectronic devices such as photodiodes and especially Quantum size effects caused by the spatial confinement of electrons Finite grain delocalization [4] Several processes make it possible to ensure the deposition of the films in our presentation of the seminar we will talk about the chemical and physical processes and we will explain in particular the processes of electrodeposition.

Keywords: Electrodeposition, Nanostructures, Materials.

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Effect of aluminum doping on electrical properties of ZnO : $Al/p-Si$ heterojunction

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Abstract. In this paper, the electrical properties different diodes were reported. Pure and Al-doped ZnO thin films of different concentrations (Al: 1, 2 and 3wt.%) were deposited by sol-gel dip-coating onto p-Si substrate to form heterojunctions [1–4]. Zinc acetate dehydrate, hexahydrate aluminum chloride, ethanol and ethanolamine were used as a starting material, doping, solvent and stabilizer, respectively. The dip-coating process with drying was repeated 6 times to obtain multilayer films.The morphological and electrical properties of the thin films as a function of Al concentration have been investigated using atomic force microscopy (AFM) and current-voltage (I-V) measurements at room temperature. AFM images revealed that grain sizes and surface roughness increase with increasing Al concentration. I-V characteristics of the diodes exhibited high and low currents under forward and reverse bias, respectively. The ideality factors (n), rectification ratio (RR) and barrier heights (BH) were found to range from 1.97 to 8.34, 0.84 to 5958 and 0.80 to 0.86 eV for different Al doping concentrations, respectively. These findings showed no monotonic behaviour of the calculated parameters with varying Al doping concentrations. The best electrical characteristic was obtained for the sample n-ZnO: 2 % Al/p-Si with an ideality factor of 1.97 eV, reverse-saturation current of 1.69E-08 A, rectification ratio of 5958 at ± 2 eV, and barrier height of 0.85 eV.

Keywords: AZO, Silicon, Heterojunction, Dip-coating, Electrical properties

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9 New magnetic materials (NMM)

9.1 Plenary Session

Theoretical investigations study of structural, mechanical and Optoelectronic Applications of ternary semiconductors $YAgTe_2$ under high pressure

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Abstract. For the moment, several studies are directed towards the use of ternary materials of group I-III-VI2 which crystallize in the chalcopyrite structure, these compounds have attracted the attention of physicists because of their wide technological applications (cells solar cells[1, 2], light-emitting diodes, detectors[3]. In the present work, structural, electronic, mechanical, elastic and optical properties of compound $YAgTe_2$ in tetragonal and chalcopyrite (P421m and I42d) respectively. has been performed by density functional theory (DFT).Based on the generalized gradient (GGA) approach, the stability accompanied with the structural parameters of the studied structure compounds was evaluated. Furthermore, modified Becke-Johnson exchange potential (TB-mBJ) was adopted for the exchange correlation potential in order to prove the electronic and optical features of $YAgTe_2$. For the P421m structure, the lattice parameters found are very close to those of the experimental and theoretical parameters. This study showed that $YAgTe_2$ is elastically stable in the two studied structures (P421m and I42d). Electronic properties showed that $YAgTe_2$ is a semiconductor in all studied structures with a direct band gap for those indicating that our compounds possess promising semiconductor behavior for photovoltaic applications. Elastic properties of $YAgTe_2$ the shear modulus, the Young's modulus, the elastic constants, the Poisson's ratio, the shear anisotropy factor are studied. Optical properties such as dielectric function, refractive index, dielectric function were calculated in the range of 0 to 40 eV, these results highlight the optoelectronic importance of this compound.

Keywords: $YAgTe_2$, Density functional theory, semiconductor ,Phase transitions, refraction, Absorption.

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DFT study of the structural, electronic and optical properties of the CoFeRuSn Quaternary Heusler compound

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Abstract. ttttttThe quaternary half Heusler [1] alloy CoFeRuSn, which has a face-centered cubic (FCC) crystal structure and conforms to F 43m space group, has been investigated using Generalized Gradient Approximation (GGA) and mbj-GGA [2] . in the Density Functional Theory (DFT) as implemented in Wien2k [3]. We present a systematical study of the structural, electronic and optical properties of CoFeRuSn by using ab-initio calculations [4]. The structural optimization was carried out in three phases i.e. Y1 , Y2 and Y3 [5] . Energetically Y1 was found to be a stable state. The electronic structure calculations show that this compound exhibits a gap in the minority states band and is clearly a half-metallic ferromagnet. In addition, the density of state is presented to show the various contributions of elements orbitals to valence and conduction bands. Also, optical properties like dielectric function, reflectivity, energy loss function, absorption coefficient and optical conductivity were calculated.

Keywords: heusler, DFT, half-metalic, Wien2k.

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HOMO-LUMO, GLOBAL CHEMICAL REACTIVITY DESCRIPTORS AND NONLINEAR OPTICAL PROPERTIES OF 1-BENZYL-5- METHYL•INDOLINE-2,3-DIONE

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Abstract. Organic compounds as isains and its derivatives have special properties due to the versatility of the carbon atom, which can engage in various types of bonding - stable by hybridization - either between carbon atoms or with atoms of other elements. They are a good candidate to create compounds with remarkable optoelectronic properties and those with nonlinear optical (NLO) ones [1,2]. The importance of the NLO properties of molecules depends on their first-order hyperpolarizability [3]. 1-Benzyl-5-methylindoline-2,3-dione (BMID) is an organic crystal whichhas been characterized by monocrystal x-ray diffraction. Theoretical investigations of the compound mentioned above were performed through the use of density functional theory (DFT) with B3LYP functional and 6-311G(d,p) basis set. HOMO, LUMO and their energy gap were computed. The small HOMO-LUMO energy gap demonstrate the high charge mobility in the titled compound. Additionally, the global chemical reactivity descriptorsas the chemical potential, electronegativity, global hardness and softness and index of electrophilicity were calculated from HOMO and LUMO energies. The nonlinear optical parameters as dipole moment, mean polarizability and first-order hyperpolarizability were investigated. The high value of first-order hyperpolarizability indicates that our BMID compound has a considerable NLO characte

Keywords: Material, Organic, DFT, Energy, Orbital, NLO.

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THEORETICAL STUDY OF CHARGE TRANSFER, CHEMICAL REACTIVITY AND NONLINEAR OPTICS APPLICATION FOR A NEW ORGANIC MOLECULE

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Abstract. Thiazolidinones derivatives containing one or two five membered rings are important class of synthetic organic materials. These heterocyclic compounds are also known to exhibit a push-pull effects and nonlinear optical (NLO) applications[1]. Recently, intramolecular charge transfer in aromatic push-pull molecules has been a subject of interest in several experimental and theoretical studies [2]. Moreover, the knowledge of the crystal structure of these compounds is crucial for understanding the related charge transfer phenomena. On the other hand, the interest for NLO properties of $\pi^{\smile}$ conjugated and functionalized organic compounds has greatly increased due to their potential applications in optoelectronics [3]. Indeed, incorporation of heteroatoms (N, O, S etc.) into the chromophore brings higher thermal stability, chemical robustness and may also act as source of auxiliary donors or acceptors. From this perspective and among organic materials, thiazolidinones derivatives are very promising molecules for the study of second order nonlinear optical properties [4]. For this purpose, we have chosen 2-thioxo- 3N-(2-methoxyphenyl) -5 [4' -methyl -3'N -(2'-methoxyphenyl) thiazol-2' (3'H)-ylidene] thiazolidin-4-one, which appears a good candidate for NLO applications. Besides investigating charge transfer within this molecule, we have examined other molecular properties such as HOMO-LUMO orbitals, global reactivity descriptors and molecular electrostatic potential of the title compound. Finally, the NLO activity of the molecule is computed.

Keywords: Heterocyclic, DFT, Chemical reactivity, HOMO-LUMO, NLO.

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9.3 Poster

9.3.1 ENERGY EFFICIENCY ISSUES FOR THE DEVELOPMENT OF DIFFERENT CLIMATE SITES

ENERGY EFFICIENCY ISSUES FOR THE DEVELOPMENT OF DIFFERENT CLIMATE SITES

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Abstract. Because of the various crises facing humanity, especially from the energy side, the concept of energy efficiency has played a central role in formulating the strategic policies of countries, both in terms of energy security, food security and health security, without forgetting its impact on the climate. Energy efficiency of a family residential house when exposed to all climatic zones of Algeria. Our country has a variety of climatic zones. To do this, we base ourselves on the Köppen Geiger world map which is a reference and is constantly updated, it provides a classification of climates based on precipitation and temperature. Unlike the rest of the country, which is characterized by a desert climate, the northern part is under the influence of the Mediterranean climate. Although there are transitional climates between these two main types of climate, especially the semi-arid climate which causes severe drought in certain periods, even outside the summer season. Algeria is also a country in the subtropics where the climate is hot and dry. To cover all possible cases, the selection of the eligible regions has been limited to seven climatic zones distributed over the entire Algerian territory. Northern Algeria is a temperate region. Its climate is similar to that of other Mediterranean countries. The high plateaus are terrain bordering Tell Atlas to the north and the Saharan Atlas to the south, and the climate in certain periods is similar to that of the Sahara. In a desert climate, temperatures can exceed 44 degrees Celsius.

Keywords: energy efficiency, climatic zones, climates, temperatures, precipitation.

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Numerical simulation of the effect of temperature on the performance of a GaSb-based TPV cell

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Abstract.

Abstract: The intensive research to develop reliable and efficient thermo-photovoltaic (TPV) cells has led researchers to focus on new materials. Knowing that these cells use infrared thermal radiation, it was necessary to use new materials, especially III-V compounds. Among these materials, the binary alloy (GaSb), which is characterized by a band gap energy of about 0.72 eV (1.72 μ), is perfectly adapted to the infrared spectrum from the sun or any hot objects. In this work, our objective is to optimize performances of the multi-junction based device, InGaP/GaSb-GaSb/Si, by performing a numerical simulation with the PC1D 6. The calculation is carried out by considering temperatures in the range 200K - 300K and a global standard illumination AM1.5G. The dark current densities, the photo-current densities as well as the figures of merit (V_{oc}, J_{sc}, FF and η) are analyzed for the temperatures, mentioned above calculation code. Our results showed a slight degradation of the performance of the thermo-photovoltaic cell, due to the decrease of the open circuit voltage (V_{oc}). The short circuit current density (J_{sc}) being almost constant.

Keywords: GaSb, thermo-photovoltaic cell, conversion efficiency, temperature.

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Electrical and optical behavior of an InAsSb based nBn structure for infrared conversion

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Abstract. Applications like thermal imaging, quality control in industrial processes, medical diagnosis, night vision and thermo-photovoltaic conversion require devices equipped with infrared radiation converting components, operating between 3 μm and 5 μm. These components could be realized by using antimonide based material such as GaSb and its ternary and quaternary alloys. Devices operating in the infrared spectra suffer from high dark currents, due to the low band gap energies of the cited materials. The excess dark currents are due to excess excited carriers because of the thermal agitation. For efficient devices, it is important to limit these currents and a possible solution is to use a component's design other than the classical p-n homojunction or heterojunction. In this work, we present the electrical and optical characteristics of a new device architecture called nBn, using the InAsSb(n)/AlAsSb/InAsSb(n) semiconducting system in order to realize a thermo-photovoltaic cell. In this structure, the InAsSb compound, with an energy band gap of about 290 meV, acts as a conversion zone. The AlAsSb compound acts as a barrier, with a band gap energy of about 1.67 eV. In such design the electrical transport by minority carriers is facilitated and the device performances are improved

Keywords: InAsSb, AlAsSb, nBn, dark currents, thermo-photovoltaic conversion.

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Effect of defects on the performances of a TPV cell using InAsSb as active material

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Abstract. In the field of micro-Optoelectronics, components based on semiconductors often present average performances due to the presence of defects caused by the fabrication processes. This is the case of components using materials with low band-gap energies, particularly antimonides. In this work, we are interested in the effects of defects in a thermo-photovoltaic cell using p-doped and n-doped GaSb layers as contacts, a GaAlAsSb(p)/GaAlAsSb(n) homojunction as a barrier and an InAsSb ternary layer as an active zone. The simulation using the SCAP-1D program showed parabolic variations of the photovoltaic parameters like the open circuit voltage V_{oc}, the short circuit current J_{sc}, the fill factor FF and the conversion efficiency η. The study was carried out for different energy levels of defects and different concentrations, in the InAsSb ternary layer. A strong degradation of the cell performances is noted for a defect density greater than 1013 cm^{-3}. This is mainly due to the degradation of the open circuit voltage

Keywords: InAsSb, thermo-photovoltaic cell, defects, GaSb.

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Electrical and optical behavior of an InAsSb based nBn structure for infrared conversion

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Abstract.
Applications like thermal imaging, quality control in industrial processes, medical diagnosis, night vision and thermo-photovoltaic conversion require devices equipped with infrared radiation converting components, operating between 3 μm and 5 μm. These components could be realized by using antimonide based material such as GaSb and its ternary and quaternary alloys. Devices operating in the infrared spectra suffer from high dark currents, due to the low band gap energies of the cited materials. The excess dark currents are due to excess excited carriers because of the thermal agitation. For efficient devices, it is important to limit these currents and a possible solution is to use a component's design other than the classical p-n homojunction or heterojunction. In this work, we present the electrical and optical characteristics of a new device architecture called nBn, using the InAsSb (n) / AlAsSb/ InAsSb (n) semiconducting system in order to realize a thermo-photovoltaic cell. In this structure, the InAsSb compound, with an energy band gap of about 290 meV, acts as a conversion zone. The AlAsSb compound acts as a barrier, with a band gap energy of about 1.67 eV. In such design the electrical transport by minority carriers is facilitated and the device performances are improved [1–3].

Keywords: InAsSb, AlAsSb, nBn, Darkcurrents, Thermo-photovoltaic conversion.

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10 Plasma and conductive energy (PCE)

10.1 Plenary Session

10.2 Oral session

10.2.1 *Experimental study of the electrical and optical characteristics of plasma controlled by a dielectric discharge barriers for UV light emission*

Experimental study of the electrical and optical characteristics of plasma controlled by a dielectric discharge barriers for UV light emission

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Abstract.
The electrical and kinetic parameters of plasma generated by sinusoidal excitation using a DBD excimer lamp in a Ne/Xe mixture are analyzed in this work. Initially, the plasma was characterized experimentally using electrical diagnostic tools (current probe, oscilloscope...) and optical diagnostics. This allowed us to observe the temporal variation of the current-voltage measured for an applied voltage of 2 kV at frequency of 40 kHz and at gas pressure of 250 mbar. Then, the optical characterization was studied in order to identify the reactive species responsible for the light emissions. The objective of the spectroscopic study is to determine the mechanisms that are at the origin of creation and disappearance of excited atomic or molecular particles responsible for the emission of UVL

Keywords: Plasma, emissions, DBD, optics, electrical, experimental.

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THE INFLUENCE OF AMMONIA ON A DISCHARGE DBD of Ar

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Abstract.
Thin layer deposition has been very popular with the scientific community in recent years. This technology consists of depositing a layer of the order of a few nanometers to a few micrometers on a substrate or on the surface of a material. Currently, anti-reflective layers of hydrogenated amorphous silicon nitride (a-SiNx:H) are made from silane (SiH4) and ammonia (NH3) as precursor gases. These layers have very good anti-reflective properties for photovoltaic cells. However, there are plasmas at atmospheric pressure suitable for depositing thin layers such as discharges controlled by dielectric barriers (DBD). This work is devoted to the study of the electrical and kinetic properties of a dielectric barrier discharge used for the deposition of antireflective and passivating SiNx:H on a crystalline silicon photovoltaic cell in the Ar/NH3 gas mixture. We have developed a zero-dimensional model for the positive column (plasma) in order to illustrate the behavior of the current, of the potential in the discharge, and of the species considered, to analyze the temporal behavior of the density of the charged and excited species. In the kinetic diagram, the Penning ionization is included which contributes to obtaining a homogeneous discharge. NH3+ ions are the dominant ions in the discharge due to Penning ionization. We look at several parameters, such as the discharge current and the chemical particles in the plasma.

Keywords: NH3, simulation plasma, DBD, ionisation de penning.

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Enhanced hydrogen generation by converting pure methane using DBD plasma reactor

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Abstract. The results of zero-dimensional time-dependent simulation modeling of hydrogen production from methane dissociation using non-thermal dielectric barrier discharge plasma in a parallel plate reactor were presented in this paper. The model includes methane dissociation reaction mechanisms pathway, an electrical circuit and the zero-dimensional plasma kinetic solver ZDPlasKin. The plasma reactor was applied to the case of a pulsed voltage of 8kV at a temperature of 300 K and under atmospheric pressure. In this work, the zero-dimensional plasma kinetic model included in ZDPlasKin code was used to investigate the behavior of the discharge such as the temporal variation of electrical and kinetic parameters. The effect of these parameters on the conversion of methane and the yield of hydrogen is also studied to enrich the knowledge for the enhancement of DBD for CH4 conversion and hydrogen production

Keywords: Hydrogen production, Reaction mechanisms pathway, Dielectric barrier discharge, Conversion, Yield.

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THE ROLE OF SILANE REACTIONS KINETICS ON THE DENSITY DISTRIBUTION IN PLASMA DISCHARGES FOR SILICON DEPOSIT

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Abstract. This work is the subject of studying the characteristics of homogeneous discharges in mixed gases such as silane SiH_4 at atmospheric pressure which is used in the deposition of plasma for the photovoltaic cells manufacture. This study is based on solving equations of one-dimensional fluid model that takes into account the primary processes like excitation, ionization and radical reactions in dielectric of silane discharges can therefore adequately represent the discharge plasma. We analyze the pressure effects on the species densities (e, H, SiH_3, SiH_3^+ and SiH_2,....etc) in such discharges using this model. In the first part we start with the calculation of the plasma voltage and the applied voltage as a function of the time, the ionization and attachment rates for a given time. Our one-dimensional model has been optimized by identifying several reactions that contribute to the production and consumption of Hydrogen which show us the effect on the density and species distribution in the plasma dielectric discharge. We will also calculate the charged species densities as a function of time as well as the spatial evolution of these particles.

Keywords: tttttt.

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STUDY OF MEASURING BONE MASS DENSITY BY DUAL X-RAYS ABSORPTIOMETRY

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Abstract. The work we have done joins medical physics. We were interested in the study of the technique for measuring bone mass density (BMD) by dual-photon X-Ray Absorptiometry (DEXA) [1-5]. For this we have done in the first stage a theoretical work to understand the interest of the bone densitometry examination for the diagnosis of osteoporosis [6,7] which is a disease of the bones, as well as the principle and the physical aspects of the interaction of X-Rays with the material, passing through the production of the X-Rays and their attenuations [8-9]. The second stage of our work was done in two private medical imaging centers located in Oran Algeria, in order to carry out a clinical and experimental study, which allowed us to attend the examination of the BMD measurement by DEXA, to obtain the values of measurements on a little sample of six patients aged between 52 and 81 years, these measurements allowed us to recheck the variation of the BMD and the T-score which is an indicator parameter of the osteoporosis according to age. The results found show a gradual decrease in BMD and T-score [1] as a function of age but which is not very significant for a patient of an advanced age of 81 years.

Keywords: one mass density, osteoporosis, X-Rays, bone densitometry, dual-photon absoptiometry, T-score.

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10.3 Poster

10.3.1 Analyse électrique et cinétique d'une source plasma de photon dans le mélange Ne/Xe

Analyse électrique et cinétique d'une source plasma de photon dans le mélange Ne/Xe

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Abstract. In this work we analyze the electrical and optical characteristics of a cold DBD plasma based on experimental observations and an electrical kinetic model and by comparing experiments / models. This study is divided into two parts. The first part aims to analyze the temporal profile of the electrical parameters of a plasma source in the Ne 50%-Xe50% mixture. The structure of a homogeneous DBD is observed for a number of experimental conditions, we thus show that the assumption of a homogeneous discharge is possible. Also we explain in this first part, why, the filamentary regime of "streamer type" is much more likely, for products with an inter-dielectric distance of 100 to a few hundred torr.cm , in the neon-xenon mixture. In a second step, we will characterize the development of the landfill using a numerical model. We calculate the variation over time of the density of the species taken into account by our kinetic scheme already developed by our research team in previous works. In this second part, we have carried out parametric studies under sinusoidal power supply, the effect of voltage and pressure will be realized in order to improve the radiative efficiency of a plasma discharge (DBD).

Keywords: filamentary, observation, DBD, plasma, electrical,kinetic.

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Development and study of UV lamps in the 207 nm for biomedical applications

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Abstract.
UV light is used for a variety of purposes in industrial processes as application in advanced semiconductor treatment technologies, synthesis of new materials and the modification of material properties, in various chemical processes in medicine and biology, disinfection of industrial wastes, water, air, and in other fields. New sources are however in full development: it is about sources, called excilampes, Their creation was preceded by intensive research on the excimer and exciplex molecules and on excimer and exciplex lasers. Lamps, as artificial sources of spontaneous radiation, play an important role in medical, biomedical and dental environments, including phototherapy, fluorescent effects, curing and drying of inks and resins and tanning, DNA treatment without causing damage, removal of bacteria, disinfection, it has been used to successfully treat a number of diseases, including rickets, psoriasis, eczema and jaundice... Our work consists in making an electrical and optical study of a dielectric barrier discharge. The discharge is filled with a gaseous mixture of Krypton and Bromine for applications in the medical and biomedical field. It has been reported to be very effective in destroying bacteria and promote healing and therefore a promising adjunctive therapy for chronic wounds infected with resistant bacteria. Very recent studies show that 207 *nm* UV light effectively kills resistant bacteria such as ISO1 and MRSA2 and produces almost no pre-mutagenic DNA damage unlike conventional germicidal UV light. The biophysical justification is based on the limited penetration distance of 207 *nm* lig [1, 2].

Keywords: Dielectric barrier discharge, Exciplexes, KrB, UV, Biomedical applications.

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11 Modeling and simulation of radiation-matter interaction (RM)

11.1 Plenary Session

Mathematical modeling of the thermoluminescence (I-TL) in $SrY_2O_4:Eu^{3+}$

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Abstract. In this We present mathematical models which describe the thermoluminescence process of SrY_2O_4 doped Eu^{3+} ions. Firstly, the kinetic parameters were calculated using the glow curve deconvolution program (GCD). We have used these parameters in our program of the proposed model. The two electron traps and one kind of recombination center (2T1R) has been used to explain the TL glow curve in $SrY_2O_4:Eu^{3+}$. Finally we deduced here that the results are in good agreement with the previously published data for the SrY_2O_4 single crystal doped Eu^{3+} ions.

Keywords: .

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11.3 Poster

11.3.1 Study of the physical characteristics of sodium halides in interaction with X-rays

Study of the physical characteristics of sodium halides in interaction with X-rays

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Abstract. Given the successful experience with the scintillator material, sodium iodide NaI, in the manufacture of the detectors, the objective is to compare it with materials belonging to the same family (sodium halides), which are: NaBr, NaF, NaCl. By making a numerical study of some physical characteristics such as the linear and mass attenuation coefficient, the total effective cross-section, the effective atomic number, the effective electron number, of the behaviour of these materials when interacting with X-rays, and this thanks to the GEANT4 simulation code which allowed us to model this interaction and to collect the results of the linear attenuation coefficient of our materials of interest. And on the other hand with the help of the Nist-XCOM database and the Fortran programming software. Thus, we were able to have a comparative study that confirms the credibility of our results with the GEANT 4 code. The results obtained give good approaches to introduce new materials for X-ray detection that can be well used in different medical and industrial fields such as NaBr and to enrich our study we have performed a detailed study of sodium bromide doped with thallium NaBr(Ti) material

Keywords: Nist-XCOM, Geant 4.

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12 Modeling and analysis of COVID-19 epidemics with treatment (CE)

12.1 Plenary Session

12.2 Oral session

12.2.1 Experience of the CHUO neonatology service during the COVID 19 pandemic

Experience of the CHUO neonatology service during the COVID 19 pandemic

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Abstract.
The Covid-19 epidemic that occurred in the first half of 2020 raised many fears about the consequences of viral infection in pregnant women and their newborns. At the end of the summer, the available data did not show an increased risk of infection and complications in pregnant women compared to the general population. In the absence of severe maternal involvement, those concerning the fetus and the new born were also reassuring [1]. We conducted a descriptive retrospective cross-section a analytical study during the month of August 2021 The sample consists of 24 newborns from a COVID-19 positive mother. Average age of mothers: 30 years old. 9 term births and 15 premature births including 3 very premature babies. 01 single Twin pregnancy after 27 weeks. 21 births by high way and 02 by low way. 04 mothers hospitalized in intensive care, 03 deceased and 01 saved. he predominant symptom in newborns is respiratory distress (75 %).02 new borns presented a fever. PCR not done in all newborns due to lack of technical platforms. 2 serologies done, one: IGM + IGG + and the other: IGM – IGG +. 04 very premature babies benefited from non-invasive ventilation (nCPAP) + surfactants deceased. Favorable evolution for the rest of the NN after an average hospitalization of 04 days. Several cases of neonatal SARS-CoV-2 infections have been reported worldwide to date. The clinical picture seems less severe and neonatal mortality linked to COVID 19 has not been reported to date. It is difficult to precisely describe the symptom at ology presented by newborns because studies do not systematically distinguish them from others infants under one year old. The clinical picture presented by the premature newborn was completely non-specific: respiratory distress with ventilatory support in the context of a pre-existing disease of the hyaline membranes and brady-apneic syndrome of the premature. However, the absence of fever in this case. At present, very few arguments in favor of maternal-fetal (so-called vertical) transmission have been found in the literature. PCR was not always available to confirm or rule out COVID-19 infection in newborns, however in our series the results are the same observed worldwide.

Keywords: Covid-19, Newborns, SARS-CoV-2

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Controlling COVID-19 outbreak in Algeria using meta-heuristic optimization algorithm

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Abstract. In this paper an efficient mathematical model called DZ-COVID-19 is proposed, due to its simple design, it can be used easily to modeling and predicting the COVID-19 outbreak in our country Algeria. The proposed DZ-COVID-19 model, depends basically on two main parameters, The reproduction number R_0: the average number of secondary cases each case generates and the serial interval S_I, this two parameters are adapted by two new weighting factors α and β in function of time t, in order to enhancing the nonlinearity behavior of the model, to make it gives precisely results for predicting the incidence infections in the coming weeks in order to help the responsible to make decision. The four parameters R_0, S_I, α and β is estimated optimally based on a recent algorithm of artificial intelligence (AI) inspired from nature called Grey Wolf Optimizer (GWO) using MATLAB language software.

Keywords: Coronavirus, COVID-19, Algeria outbreak, DZ-COVID-19 model, Grey Wolf Optimizer, A mathematical model.

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12.3 Poster

12.3.1 *Numerical model of two-phase flow in the pulmonary bronchi for the treatment of the covid-19 pandemic*

Numerical model of two-phase flow in the pulmonary bronchi for the treatment of the covid-19 pandemic

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Abstract.
COVID-19 may cause respiratory distress syndrome (RDS), the leading cause of mortality in patients. However, surfactant replacement therapy has been an integral part of the management of this distress. The main objective of the present work is to study the phenomenon of two-phase flow in the presence of two different surfactants (Curosurf and Infasurf) in the airways and deduce which of them gives us a more homogeneous distribution. By using the CFD tool, the solution of Navier-Stokes equations, and the calculation of homogenization and efficiency were performed. We carried out a simulation of surfactant instillation with realistic models of human airways on the real geometry of the superior part of the tracheobronchial tree 4th generation (the trachea up to the 16th branch) by using the commercial software ANSYS FLUENT (19, 22) as well as refined mesh based on tetrahedrons with mesh step e-3. This simulation provided several contour profiles of different pressures, velocities, volume fractions and others for the two surfactants in the 16 outlets of the geometry. Our study may suggest choosing Curosurf surfactant, which is better than Infasurf surfactant [1–3].

Keywords: Covid-19, respiratory distress syndrome (RDS), surfactant replacement therapy, surfactant, Infasurf, Curosurf.

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