6th International Conference on the World of Technology and Advanced Materials

23-24 October 2023

BOOK OF ABSTRACTS

Faculty of Matter Sciences

University of Batna 1

Laboratory of Physical and Chemical Studies of Materials

(LEPCM)

BATNA 1 UNIVERSITY

FACULTY OF MATTER SCIENCES

LABORATORY OF PHYSICAL AND CHEMICAL STUDIES OF MATERIALS (LEPCM)

6th International Conference on the World of Technology and Advanced Materials

23-24 October 2023

WITAM'23

BOOK OF ABSTRACTS

PREAMBLE

The Laboratory of Physical and Chemical Studies of Materials (LEPCM) and the Faculty of Matter Science of Batna 1 University organize the sixth International conference on the Thermodynamics of Metallic Alloys in Batna (Algeria) on 23 and 24 October 2023.

This conference is a forum where Algerian and foreign researchers meet, know each other, make known to young researchers their fields of research, present their work, weave or consolidate the relations of cooperation between their different research structures (groups, laboratories, units, centers… of research) and discuss research perspectives

This conference is also an opportunity to researchers who want to make the thermodynamics of metals and alloys as theme of reflection and see its enormous scientific, technological and industrial interest. We therefore hope that it will be of great value to young researchers and PhD students working in the fields of metallurgy, physics and chemistry of metals and their alloys.

This collection contains all the abstracts submitted and selected for the WITAM 2023 where the topics of this edition are:

1. Thermodynamic assessment and phase diagrams (CALPHAD approach).
2. Ab-initio Calculation of thermodynamic properties.
3. Experimental methods of metallic alloys characterization.

This conference also includes the participation of Professor Abdelhafid Aourag, General Director of Scientific Research and Technological Development in Algeria, with the opening plenary talk. This honors us all and it is an important encouragement to the organizers and all participants.

On behalf of the Scientific Committee, the Organizing Committee and the members of the LEPCM laboratory, we extend our heartfelt thanks to the Rector of Batna1 University, Professor Dif Abdesslem and the Dean of the Faculty of matter science for their unconditional support of this conference. These thanks also go to all the participating researchers and sponsors whose financial contribution has contributed to the success of the organization of this scientific event.

We wish everyone a pleasant stay in Batna and success of this conference.

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PLENARY TALKS

HOW TO ACCELERATE THE DISCOVERY OF NEW MATERIALS?

H. Aourag

SMRIS, CRTI, Oran, Algeria

Abstract :

The earth and humanity are in danger and we are all responsible.Our planet is burning and we look elsewhere. Nature, mutilated, overexploited, is no longer able to reconstitute itself and we refuse to admit it. Humanity is suffering from starvation, natural catastrophe, pandemic... It suffers from poor development of new solutions and specifically of new materials which could overcome this situation.

Materials discovery is a complex process that involves the prediction, synthesis and characterization of new materials. This requires a thorough understanding of the interaction between the atomic and electronic structures of materials and their properties. Currently, this process is largely guided by trial and error, and the computational models used to predict material properties are often inaccurate or incomplete and this processes need several years to discover a new effective material.

Materials discovery is a complex process that involves the prediction, synthesis and characterization of new materials. This requires a thorough understanding of the interaction between the atomic and electronic structures of materials and their properties. Currently, this process is largely guided by trial and error, and the computational models used to predict material properties are often inaccurate or incomplete and this processes need several years to discover a new effective material.

In this plenary talk we will give a global view of the more recent approaches and techniques used to accelerate the discovery of new materials, with the more prominent results.

OPTIMIZATION OF THE HEAT CAPACITIES OF SPHALERITE PHASES AS SINGLE SYSTEM OR HOW NUCLEAR PHYSICS HELPS CHEMISTS

V.P. Vassiliev

Lomonosov Moscow State University, Chemical Department,119992, Moscow, Russia,

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valeryvassiliev@yahoo.fr

Abstract:

To describe the set of the isostructural experimental data $C_p(T)$ of diamond-like phases in solid state as a single system was used multiparameter family of functions in the form(1)

σ^2 (a, b, T_0, Θ_1, Θ_2, A_1, A_2) = $\sum_{i=1}^{n}(C_{p,calc} - C_{p,exp})^2$/n, where the coefficientsa, b, T_0, Θ_1, Θ_2, A_1>0,

(A_2=1- A_1>0),are the adjustable parameters.Parameters a, b, T_0, Θ_1, Θ_2, A_1 can be represented graphically vsLn(N).

The search for the minimum of σ^2 was carried out by three methods: the golden ratio, conjugate gradient and coordinate descent. All coefficients (a, b, T_0, Θ_1, Θ_2, A_1) can be described by polynomial equations vs Ln(N), where N is atomic number of the element of IV group (Si, Ge, α-Sn, diamond-like Pb, Fl) or demi sum of the atomic number of the $A^{II}B^{VI}$ or $A^{III}B^{V}$ phases. In this case, either a break point or an inflection point attributable to germanium is observed on the parameter *vs*Ln(N) curves.The unknown coefficients of the multiparameter function of the Al, Ga, In, Tl and Nh nitrides with ZnS structure were found by interpolation.

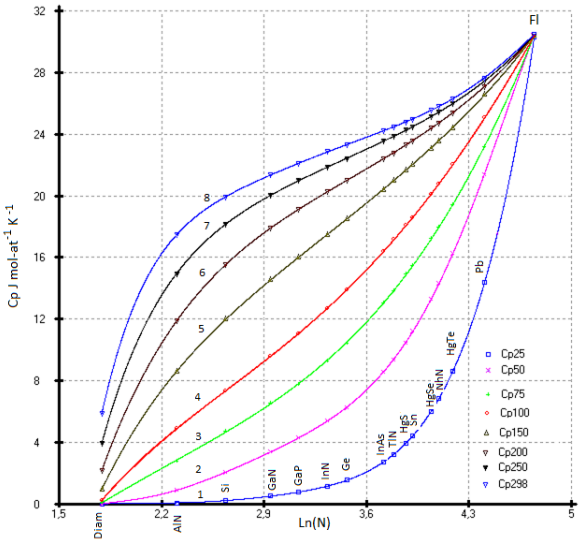

Fig.1. Isotherms of the heat capacities phases (Cp) with diamond like structure vsLnN: 1-25K, 2-50K, 3-75K, 4-100K, 5-150K, 6-200K, 7-250K, 8-298K, calculated with our model [this work].

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[2] V. P. Vassiliev. Optimization of the heat capacities of diamond-like compounds.J. Mater. Sci. Eng. B 11 (**2021**) 76-80. doi: 10.17265/2161-6221/2021.4-6.004

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ELECTRONIC AND OPTICAL PROPERTIES OF 2D MATERIALS

G. Uğur[1,], Ş. Uğur[1], M. Güler[2], E. Güler[2]*

[1]Gazi University, Department of Physics, 06500 Ankara, TURKEY
[2] Ankara Hacı Bayram Veli University, Department of Physics, 06900 Ankara, TURKEY

** G. Uğur: gokay@gazi.edu.tr*

Keywords : 2D materials, band structures, semiconducting properties, optical properties.

Abstract :

With the rapid development of nanoscience and nanotechnology, 2D (two-dimensional) materials have attracted great interest in recent years. These materials have structural properties of only two atoms thick and highly long in one dimension. The best-known examples of two-dimensional materials are graphene and thin deposition layers. This summary examines the electronic and optical properties of 2D materials, highlighting the potential of these materials in future applications [1]. The electronic properties of 2D materials include specific structures and electronic band structures. Some 2D materials, like graphene, have inherently semiconducting properties and high carrier mobilities, allowing electrons to move at high speeds. This is an essential advantage for high-speed transistors and nano-electronic devices [2]. However, some 2D materials, especially transition metal tellurides, have different energy band structures, leading to different electronic properties. For example, it has been shown that some 2D materials can act as topological insulators and can be used in spintronic applications. The optical properties of 2D materials are also of great interest. These materials show absorption and emission properties at various wavelengths. In particular, thin deposition layers can be used as optical waveguides, leading to critical applications in optical communication systems and sensors. Some 2D materials show quantum confinement effects because they comprise a single layer of atoms, which should be considered, especially in optoelectronic applications. 2D materials can control the emission or absorption of a single photon, enabling the development of single-photon devices. The electronic and optical properties of 2D materials have great potential in various applications. These materials can have different electronic properties, such as semiconductors, insulators, and metals, enabling the development of various electronic devices. They also have significant uses in several fields, such as optical communications, sensors, and photonic applications. In the future, extensive research on synthesizing and characterizing 2D materials will enable these materials to find more applications. Further, a better understanding of the fundamental properties of these materials will support the design and development of future technology. Therefore, the electronic and optical properties of 2D materials are of great importance for scientific research and technological development and are believed to become more prevalent in the near future.

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A COMBINED THEORETICAL AND EXPERIMENTAL STUDY FOR NOVEL TITANIUM BASED BIOMATERIALS

E. Güler[1], M. Güler[1], Ş. Uğur[2] and G. Uğur[2]*

[1]Ankara Hacı Bayram Veli University, Department of Physics, 06900 Ankara, TURKEY
[2]Gazi University, Department of Physics, 06500 Ankara, TURKEY

……

** E. Güler: eguler71@gmail.com*

Keywords: Biomaterials, Ti-Nb, Ti-Nb-Ge, mechanical properties, low Young modulus.

Abstract:

A combined theoretical and experimental study for novel titanium-based biomaterials was designed and performed for Ti-x%Nb-y%Ge (wt. %) ternary alloys. Theoretical studies were carried out within the density functional theory (DFT) framework, where experimental works include scanning electron microscope (SEM) observations, X-ray diffraction (XRD) analyses, and Vickers microhardness measurements. Obtained results from theory and experiments for different compositions of Ti-Nb-Ge ternary alloys with Nb < 20% wt. compositions suggest novel biomaterials with low Young modulus compatible either with the human cortical bone or tooth dentin, depending on the Ge% concentrations.

DEVELOPMENT OF NEW THERMOELECTRIC POWER GENERATION MATERIALS

Z. Charifi[1,2,*]

[1] *Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria*

[2] *Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria*

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** Corresponding author: e-mail: zoulikha.charifi@univ-msila.dz*

Keywords: electronic structure; doping, thermoelectric materials; figure of merit; Seebeck coefficient.

Abstract:

This talk provides an overview of thermoelectric materials research, covering current knowledge and recent advances. The main goal in this research is to improve the thermoelectric figure of merit (ZT) by either increasing the power factor or reducing thermal conductivity. To enhance the power factor, we work on developing new materials and enhancing existing ones through doping. To lower thermal conductivity, we employ techniques like Alloying, using Complex Structure Multiple Sites, Large Unit Volume, Heavy Atoms, and using materials with naturally low thermal conductivity. The discussion also explores bulk materials, examining their chemistry, crystal structures, physical properties, and methods for optimizing their thermoelectric performance.

SOLIDIFICATION OF METALS AND ALLOYS: BENCHMARK EXPERIMENT & NUMERICAL SIMULATION

L. Hachani

Physical Materials Laboratory (LPM); Amar Telidji University,Laghouat; BP 37 G Boulevard des Martyrs -03000 Laghouat/Algeria.

** l.hachani@lagh-univ.dz*

Keywords : Solidification, Segregation, Electromagnetic Stirring, Thermosolutal Convection.

Abstract :

This work is situated in the prospects of solidification control of the metallic alloys under the effect of natural and forced convection, in order to enhance the control of solidification process through an effective electromagnetic stirring to have a controlled magnetohydrodynamic flow in the liquid which canlead to improve the final macrostructure of the alloyand subsequentlyreduce or even completely eliminate the defects related to the segregation. The possibility considered in this work is to achieve this stirring without contacting the bulk (alloy in fusion) and pollution by other elements using a stirring by the Lorentz force. The purpose of the work consists both a numerical analysis and experimental investigations based on a Benchmark setup particularly documented and instrumented developed in SIMAP/EPM laboratory in Grenoble, named AFRODITE. The experimental device used to provide quantitative and qualitative data on the process of solidification of metallic alloys. These data are necessary for the contribution to studies on the solidification of metallic alloys and enrich the data base of numerical models developed to predict defects related to solidification. The alloy selected from our work is tin-lead, for its low melting temperature. The experiments performed are designed to study the effect of two types of dynamic configuration on the solidification of Sn-Pb alloy: the thermosolutal convection with the variation of two essential parameters (cooling rate and the difference in experimental temperature) and forced convection by the use of several modes of electromagnetic stirring. This study is particularly interested in the characterization of macrostructures and defects related to macrosegregation. Moreover, a 3D numerical model was proposed based on the enthalpy approach (to treat cases of solidification of metal alloys with the segregation phenomenon) under the influence of natural convection and forced convection caused by electromagnetic stirring. This model has been applied in order to better understand, master and control the solidification process of metallic alloys, in terms of defects that occur during the solidification, particularly segregation at the meso and macroscopic scale. The developed numerical model was validated by in-situ and real-time measurements of temperatures at any point of the solidification system, which allows quantitative and qualitative validation.

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ORAL PRESENTATIONS

EFFECT OF CALCINATION ON STRUCTURE AND PHOTOCATALYTIC PROPERTY OF Fe- DIATOMITE HYBRID PHOTOCATALYST FOR IMPROVING REDUCTION OF TEXTILE DYE

W. Rezig [1,] M.D. Hadjel [2]*

[1] Laboratory of Sciences, Technology and Process Engineering ; Department of Chemical Engineering ; Faculty of Chemistry ; University of Sciences and the Technology of Oran Mohamed Boudiaf USTO-MB ; BP 1505 El M'naoueur Bir El Djir 31000 Oran ; Oran ; Algeria.

[2] Laboratory of Sciences, Technology and Process Engineering ; Department of Physical Chemistry ; Faculty of Chemistry ; University of Sciences and the Technology of Oran Mohamed Boudiaf USTO-MB ; BP 1505 El M'naoueur Bir El Djir 31000 Oran ; Oran ; Algeria.

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** Corresponding author: walidrzg@gmail.com*

Keywords : Silica, hematite, nanoparticles, Iron, gap band.

Abstract :

Silica coated hematite nanoparticles " SCHN " composite as catalyst and characterized in this study. SCHN was made a surface modification treatments including Iron (III) nitrate nanohydrate $Fe(NO_3)_3.9H_2O$ deposition on raw diatomite .In the $Fe(NO_3)_3.9H_2O$ treatment,surface silica of diatomite and TiO_2 degussa P25 were partially dissolved in The iron (III) nitratenanohydrate $Fe(NO_3)_3.9H_2O$ by means of x-ray fluorescence (XRF), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and UV-visible diffuse reflectance spectroscopy (DRS).The surface area of SCHN is 855 m^2/g.The surface modification also increased the point of zero charge (pH_{PZC}) values to 6 for Silica coated hematite nanoparticles with gap band was Eg= 1.1 eV by UV-visible DRS technique. The colour removal of vat green 03 indanthren in different pH's using the diatomite modified TDF. It was observed that the vat green 03 indanthren textile dye degradation has pH dependency ,the better result is at pH = 10.

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CALCULATION OF THE ACTIVATION ENERGY OF CRYSTALLIZATION OF NANOSTRUCTURED TiAl ALLOY PRODUCED BY MECHANICAL ALLOYING

S. Triaa[1], F. Kalli-Ali[1] and S. Taane[1]*

[1] Laboratoire des sciences et génie des matériaux (LSGM),

Université des Sciences et de la Technologie Houari Boumediene, BP 32 El Alia 16111, Alger - Algérie.

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** Correspondant : striaai@usthb.dz et salimtria@yahoo.fr*

Keywords : Ti-Al alloy, activation energy, crystallization kinetics parameter, DSC

Abstract :

The crystallization procedure of TiAl metallic alloy elaborated by high-energy ball milling investigated by Differential Scanning Calorimetry (DSC) and X-ray diffraction methods. The crystalline phase of Ti-Al alloy was identified during the primary crystallization process.

The activation energy of crystallization *'Eα'* has been calculated using the Kissinger and Ozawa model. The activation energy for crystallization of $Fe_{64}Cr_{36}$ alloy was determined at various heating rate of 5, 10, 20 and 30 K min^{-1}.

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CALPHAD MODELING OF INTERMEDIATE PHASES BASED ON TWO SUBLATTICE MODEL

H. Ghamr[*]

Laboratory of Physical and chemical studies of materials (LEPCM)Physics, Department, Faculty of Matter Sciences, University of Batna1, Algeria

** Corresponding author: houda.ghamri@univ-batna.dz*

Keywords : Calphad, intermediate phases, sublattice model, Wyckoff sites.

Abstract :

The sublattice model[1, 2] is one of the most commonly used Gibbs energy models in the Calphad modeling. It was constructed in order to describe the thermodynamic properties of intermediate phases which show a solubility range.It consists in dividing the phase into the different sublattices.Crystallographic information is mainly used for deciding the number of sublattices to be used, for assigning constituent species (including possible vacancies) to each of them and defining the nature ofthe disorder (anti-site atoms, vacancies or interstitials) necessary to accommodate the non-stoichiometry.

For development of a good model description, the crystallographic sublattices must be taken into account, where initially one sublattice is assigned to each Wyckoff position and the site occupation is noted. The multiplicity of the site becomes the stoichiometric factor of this sublattice. The second step is to examine how these occupations change on deviation of stoichiometry, i.e. whether substitution occurs, vacancies are found or interstitials are formed.The crystal structures of many phases in metallic systems are fairly simple and may have only three or fewer Wyckoff sites. However, for phases with complex crystal structures which have four or more Wyckoff sites, it is often necessary to avoid too many end-membersbycombining two or more of the Wyckoff sites into one sublattice.

When selecting a sublattice model for a phase, due credit must be given to known crystallographic and solubility range data for the phase, not only in the system under consideration, but also in other systems (binary as well as higher-order) where the same phase is observed.

This work gives a brief introduction to the sublattice model and then provides a set of examples of how thermodynamic modelling has been successfully used in describing intermediate phases such as B1, C15 and C36 in some binary systems by the two-sublattice (2SL) model.

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EXPERIMENTAL INVESTIGATION OF PHASE DIAGRAMS INTHE Sb-Sn SYSTEM

A. Rahmouni, A. Belgacem Bouzida and Y. Djaballah

Laboratory of Physical and Chemical Studies of Materials (LEPCM), Physics Department, Faculty of Matter Sciences, University of Batna 1, Algeria, 05000, Algeria.

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ayoub93.r@hotmail.fr

Keywords :

Phase Diagrams, Sb-Sn System, Differential Scanning Calorimetry (DSC),Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), Material Characterization.

Abstract :

Our research is dedicated to the meticulous examination of phase diagrams within the Sb-Sn system [1]. This system poses intricate challenges concerning the existence of well-defined compounds, making it a pivotal subject for comprehending its physical and chemical characteristics. Our investigative approach involves employing sophisticated techniques such as Differential Scanning Calorimetry (DSC) [1], Scanning Electron Microscopy (SEM) for microstructural phase observations [2], and X-ray Diffraction (XRD) for confirming crystallographic arrangements [3].

This comprehensive study endeavors to deliver substantial insights into the phase diagrams of the Sb- Sn system, primarily by confirming the presence of previously presumed compounds and methodically characterizing their phases. Through our experimental endeavors, we aim to contribute valuable data that will deepen our understanding of this intricate system. This understanding, coupled with athorough exploration of the system's thermodynamic properties and microstructural evolution, lays the groundwork for potential applications in diverse material science and engineering domains.

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AB INITIO CALCULATIONS OF THE STRUCTURAL, THERMODYNAMIC, ANISOTROPIC ELASTIC AND VIBRATIONAL PROPRIETIES OF THE B2-TYPE NICKEL-BASED COMPOUNDS

R. Benhafid [1], A. Belgacem Bouzida*

[1] Laboratory of Physical and Chemical studies of Materials (LEPCM),

Physics Department, Faculty of Matter Sciences, University of Batna 1, Batna, Algeria

Email : rabia.benhafid@univ-batna.dz

Ke words : Ab initio calculations, anisotropic, vibrational, B2-type, GGA approximation.

Abstract :

In this work, we have computed the structural, thermodynamic, anisotropic elastic and vibrational properties of Ni-X (X=Al and Ga) compounds. The compound NiAl (nickel aluminum nitride) is known for its high-temperature resistance and mechanical properties. The intermetallic compound B2 NiAl is widely used in aerospace applications due to its high melting temperature[1] (T = 1911 K) good oxidation resistance and low density[2].

The calculations were performed within the framework of density functional theory [3] (DFT), using the VASP (Vienna Ab initio Simulation Package) code, the foundations of which were laid by Kresse and Furthmüller[4]. The calculations employed the projector augmented-wave[5](PAW) method with the generalized gradient approximation[6] (GGA). The calculated equilibrium lattice parameters and formation enthalpy are in good agreement with the available experimental data and other theoretical results. The calculated results indicate that the NiAl and NiGa compounds are mechanically stable. Elastic properties including bulk modulus, shear modulus, Young's modulus, and Poisson's ratio are also obtained. The elastic anisotropies of these compounds are investigated via the three-dimensional (3D) figures of directional dependences of reciprocals. Finally, based on the quasi-harmonic Debye model, the heat capacity and Debye temperature of

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A NOTE IN ASSESEMENT OF BINARY PHASEDIAGRAM.

A.Ferroudj, Y. Djaballah*

Laboratory of Physical and Chemical studies of Materials (LEPCM),

Physics Department, Faculty of Matter Sciences, University of Batna 1, Batna, Algeria

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abdelhak.ferroudj@univ-batna.dz

Keywords : Calphad, binary compounds, Gibbs equation.

Abstract :

This work presents the thermodynamic theoretical part which constitutes the fundamental basis of the Calphad method which aims to establish and trace binary or ternary phase diagrams. The formalism integrated into all the diagramming programsis based on the Gibbs equation

$$G_{\emptyset} = G_{\emptyset}^{0} + \Delta G_{\emptyset}$$

$$G_{\emptyset} = \sum_i x_i \, {}^{\circ}G_i + \mathrm{RT}\sum_i x_i \ln(x_i) + G_{\emptyset}^{E}$$

The last requires certain experimental data such as enthalpy and entropy of formation,the melting temperatures of the compounds and constituents .

But are these data really sufficient for the description of all intermetallic equilibriumstates in binary systems?

In order to clarify this problem we will discuss some laws acting on the existence ofdefined compounds or their abillation.

PREDICTION OF PHYSICALS PROPERTIES OF ZINTEL COMPOUNDS Ba_2P_7X(X = Cl, Br, I)

A.Kerboub, E. Belbacha*

Laboratory of Physical and Chemical Studies of Materials (LEPCM), Faculty of Matter Sciences, University of Batna 1, Algeria

** Corresponding author: abdelhak.kerboub@univ-batna.dz*

Keywords : Ab-initio, inter-metallics, Zintel, CASTEP.

Abstract :

In this work, we have studied the structural, elastic and electronic properties for the ternary Zintel phase compounds of the form Ba_2P_7X where (X = Cl; Br; I), which crystallize in the structure monoclinic and belong to the group P21/m. We used the ab-initio calculation method, which is that of the pseudo-potential and plane waves (PP/PW) in the frame work of the density functional theory (DFT) and implemented in the CASTEP code, by processing the Exchange energy and correlation by the approximation of the generalized gradient of Perdew- Burke-Ernzerh of GGA/PBE-sol. The equilibrium geometric of the studied materials have been optimized at T = 0K by using the CASTEP package. For a good description of the mechanical behavior of the studied compounds, we have calculated theirs single-elastic constants C_{ijs}, and from these numerical values obtained for the C_{ijs} we estimated isotropic elastic modulus and their related properties for single-crystal and polycrystalline phase, including the namely bulk modulus, shear modulus, Young modulus, Poisson ratio, elastic anisotropy indexes. As we have used the numerical values of C_{ijs} to check the mechanicals stabilities. We also discussed the electronic properties: band structure, total and partial electronic density diagrams (TDOS and PDOS) as well as electronic distribution.

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DEVELOPMENT OF A GRAPHICAL USER INTERFACE FOR VASP CODE: "LEPCM-VASPGUI"

H. Righi[1,] , M. Diaf[1]*

[1] Laboratory of Physical and Chemical Studies of Materials (LEPCM). Faculty of Matter Sciences , Department of Physics, University of Batna 1, Batna,

** Corresponding author: email: haroun.righi@univ-batna.dz*

Keywords : Vasp ,GUI,C++, Qt librairy

Abstract :

VASP (Vienna Abinitio Simulation Package) [1-3] is the most used code in the modeling of the physical properties of crystals, it is an computer code for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials . calculating the physical properties of crystals using VASP requires several processing steps pres and post data processing. LEPCM-VASPGUI presents a C++ application for data processing in order to facilitate the calculation of structural, electronic, and elastic properties. In this work we will present the different stages of use development and of our GUI using library QT [4] going from installation on linux system, to configuration and exploitation of the code. we will present calculation results on simple systems in order to make a comparison with other codes.

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SOLIDIFICATION OF AN Al-Mg ALLOY UNDER SURFACE TENSION ANISOTROPY

A. Djaraoui[1], K. Oulmi[2], D. Haddad[3]*

[1]Process engineering department, Faculty of Engineering Sciences, University Batna2, Batna, Algeria

[2]Chimics department, Faculty of Sciences, University Batna1, Batna, Algeria

[3]Health and Safety department, Faculty of Engineering Sciences, University Batna2, Batna, Algeria

**Corresponding author email: a.djaraoui@univ-batna2.dz*

Keywords : VFT Model, Surface tension anisotropy, Equiaxed dendrite, Al-Mg alloy.

Abstract :

The equiaxed dendrite morphologies, growing into an undercooled Al-8wt%Mg liquid melt with 15degree orientation are numerically simulated using the Virtual Front Tracking VFT model. Local equilibrium at the liquid solid interface are solved to simulate the 2D growth, in isothermal solidification conditions. The mechanism and kinetic of interface movement is simulated by considering the eight cells assigned as interface cells. The domain is a $200\ \mu m \times 200\ \mu m$ divided into 403×403 cells. The aim of this work is to contribute on the study of how the surface tension anisotropy coefficient variation $(0 \leq \delta < 1)$ affect the dendrite shapes and crystallographic orientation directions. The results obtained for lower degrees of thermal supercooling are in good agreement with the stability theory. For high degree supercooling, the results show a competition between the two terms (T T) and of the local equation of the interface equilibrium composition controlling the dendrite growth features.

As part of our comprehensive study, we also present a figure, which visually represents one of the results obtained, displaying the impact of different surface tension anisotropy coefficients on dendrite growth.

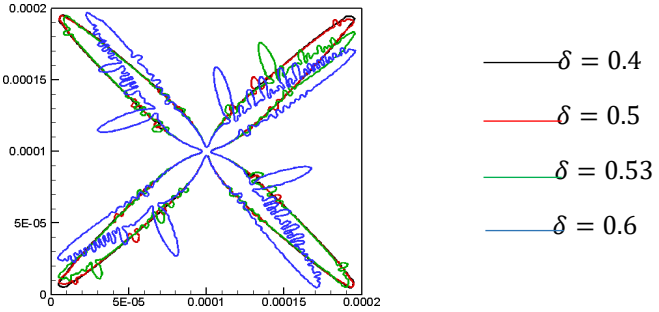

Fig. —The simulated Al-8wt% Mg dendrite at $\Delta T = 10K$, for $\Delta t = 10^{-4}s$, with $\delta = 0.4$, $\delta = 0.5$, $\delta = 0.53$ and $\delta = 0.6$, $\theta_0 = 15\ deg$ for 1s. The computational domain is divided into 403×403 cells. The capturing rule is the eight cells.

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FIRST PRINCIPLES INVESTIGATION OF STRUCTURAL,ELASTIC, ELECTRONIC AND VIBRATIONAL PROPERTIES OF DICISIUM CLORIDE PEROVSKITES Cs_2MCl_6 **(**$M = T\mathrm{i}, Mo\ \&\ Mn$).

H.Krarcha[1,2,*] *B.Bennecer*[3]

[1] *Lrpirm laboratory, Department of physics, faculty of sciences, university Batna1,Batna 05000 Algeria.*

[2] *Earth sciences &universe institute, University of Batna 2, 53, Constantine Street, Fesdis, Batna 05078, Algeria*[3]*Physics Laboratory at Guelma, Faculty of Mathematics, Computing and Material Sciences, University 8 Mai 1945Guelma, P.O. Box 401 Guelma 24000, Algeria,*

* *h.krarcha@univ-batna2.dz*

Keywords : ab initio, elastic constants, Density functional theory, perovskite.

Abstract :

and Structural, elastic, electronic and vibrational properties of cloride perovskites : Cs_2MCl_6

(M = Ti, Mo & Mn) compounds on cubic structure with space group $Fm3\ m$ structure are studied by first principles method within generalized gradient approximation. The calculated negative formation enthalpy for each perovskite confirm the thermodynamical stability of the studied phase. Band structure calculations reveal that compounds have an band gap of the range between

1.42 and 5.0 eV. We can notice from electronic calculations that the values of band gap increases by de creases of valence number of transition metal.

The calculated elastic constants and the phonon dispersion relations of the studied compounds show that these compounds are both mechanically dynamically stable. Moreover the temperature dependence of the specific heat and entropy have been calculated and discussed in details.

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VACANCY DEFECTS IN CZTS THIN-FILM SOLAR CELLS: A DFT INVESTIGATION

A. Hidoussi[1,2*] *K. Rahmouni*[3,4]

[1] *University Center of Barika, Institute of Sciences, Algeria.*

[2] *Laboratory of Physical and Chemical Studies of Materials (LEPCM), Department of Physics, Faculty of Matter Sciences, University of Batna 1, Algeria.*

[3] *ISTA, University of Larbi Ben M'hidi, Oum El Bouaghi, Algeria.*

[4] *Laboratory of active components and materials. Larbi Ben M'hidi University Oum El Bouaghi. BP 04000, Algeria.*

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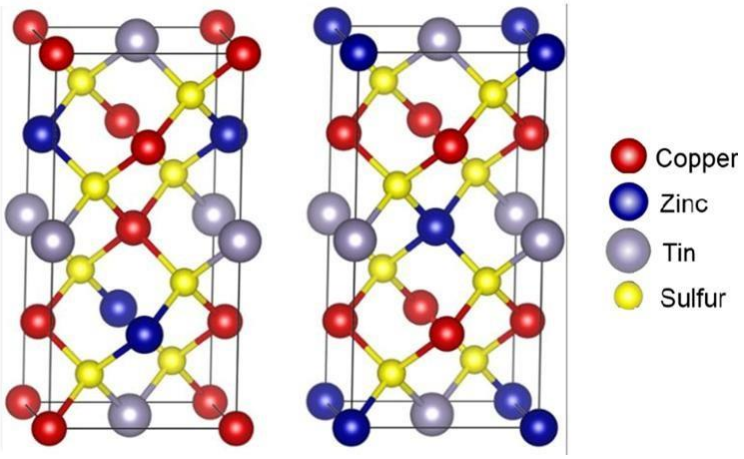
** Corresponding author: aissam.hidoussi@cu-barika.dz*

Keywords : CZTS, Thin-Film, Solar Cells.

Abstract :

Copper Zinc Tin Sulfide (CZTS) and Copper Zinc Tin Sulfur Selenide (CZTSSE) has emergedas a promising candidate for thin-film photovoltaic technology, providing an environmentally friendly alternative to Cadmium Telluride (CdTe) and Copper Indium Gallium Selenide (CIGS) due to its abundance of constituent elements, non-toxic nature, and potential for sustainable solarenergy generation. In this study, we employed Density Functional Theory (DFT) calculations to investigate the electronic properties of CZTS thin-film solar cells, with a particular focus on vacancy defects. Sulfur (S) were found to be the most favored vacancy defects. The calculated electronic properties and defect formation energies are in excellent agreement with results available in the literature.



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IMPROVEMENTS OF THE PHYSICAL PROPERTIES OF DOPED SAMARIUM MONOXIDE (SmO)

A. Bendahah, D. Bensaid, K. Bencheri

Laboratoiry of Materials Magnetic UDL SBA, Algéria Laboratoiry of Matérials & brumin Optics(LEMIO)UDL SBA, Algéria

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abila_05@yahoo.fr

Keywords: Doped semi conductor , DFT, spintronics and half- metal.

Abstract:

Rare earth compounds are now widely used in several research fields in electronics and spintronics. Ferromagnetic semi conductors based on rare earth oxides such as europium monoxide EuO or samarium monoxide SmO, whose magnetism comes from partially filled 4f states. Doping with an element d or f allows to increase Tc with a decrease in resistivity, and gives us insulator-metal transitioninduced by a change in band structure[1]. We are interested in the ferromagnitic half-metal phase of this kind of compound. We try to substitute SmO by transition elements such as Co, Sc, Ti and Cr using theDFT formalism.

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EFFICIENT CHARGE CARRIER SEPARATION ENABLED BY POLARIZATION IN POLAR Cu $_2$Se AND SOLAR HARVESTING :FIRST-PRINCIPLES INVESTIGATION

N. Chelil[1,], M.Sahnoun[1]*

[1]Laboratory of Quantum Physics and Mathematical Modeling (LPQ3M),Mascara, Algeria

** Corresponding author: n.chelil@univ-mascara.dz*

Keywords : Perovskite, photovoltaics, photocurrent, ferroelectric.

Abstract :

The efficient separation of charge carriers, driven by polarization effects, has identified ferroelectric semiconductors with narrow band gaps (~1.3 eV) as an ideal choice for the active layer in photovoltaic systems. Recent studies on lead halide perovskite solar cells have substantiated this concept. This research proposes polar Copper selenide (Cu_2Se) as a highly promising candidate for high-performance ferroelectric photovoltaics. Through density functional theory calculations, it is uncovered that Cu_2Seexhibits a moderate macroscopic polarization of 28.78 $\mu C.cm^{-2}$, which is sufficient for the separation of charge carriers. Furthermore, $Cu_2Se$is predicted to possess a direct band gap of approximately 0.99 eV. By analyzing the optical absorption coefficient and the nonlinear photocurrent shift bulk photovoltaic effect, it is illustrated that an extremely thin layer of Cu $_2$Secan generate substantial photocurrents in the visible range exceed the maximum response obtained for $BiFeO_3$ by 3 times. Superior ferroelectric properties coupled with highly reported nonlinear optical behavior makes Cu $_2$Seas a potential candidate for green energy generation.

REVEALING THE STRUCTURAL, ELECTRONIC AND MECANICAL PROPERTIES OF $Ca_{1-X}Np_XSn_3$ (X=0, 0.5,1) ALLOYS .A THEORY CALCULATION

M. Fodil[1,] , A.Touia [2]*

[1] Faculty of Science and Technology, Hassiba Benbouali University, No 19, Chlef, 02000, Algeria

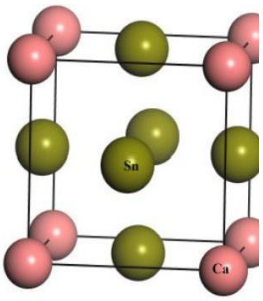
[2] Laboratory of Materials Science and applications, Belhadj Bouchaib University, BP 284, Ain Temouchent, 46000, Algeria

** maroco_mr@hotmail.fr*

Keywords : first principles, AuCu3-type crystal, Elastic properties, metallic alloys .

Abstract :

Intermetallic compounds provide a diverse and extensive field for researchers to explore connections among constituent elements, chemical interactions, atomic structure, electrical configuration, and physical properties.This work is interested to examine the characteristics of compounds Ca_{1-x} Np_x Sn_3 with values of x are : 0, 0.5 and 1. The density functional theory (DFT) method was used in conjunction with the Wein2k code[1] for analysis. The study used the generalized gradient approximation (GGA) proposed by Perdew-Burke-Ernzerhof (PBE) [2]. The compounds considered belong to the cubic structure of the AuCu3 type, as shown in Figure 1.a.In order to verify the physical properties, the bulk modulus and ground state lattice constants were optimized. some amount of energy releases can further be used in Murnaghan expression of states for the calculation of ground-state characteristics [3]. The results show that The elastic characteristics of Ca_{1-x} Np_x Sn_3 are predicted to be strongly compositionally dependent (Young's modulus, E, and shear modulus, G) , with modest levels of elastic anisotropy and a low Debye temperature response. for concentrations around x=0.50. The Ca_{1-x} Np_x Sn_3 exhibits brittleness and directed bonding properties. The electronic band structures (figure 1-b) for Ca_{1-x} Np_x Sn_3 materials show metallic conductivity in which Ca-3d /Np-6d and 5p-Sn states dominate. These orbitals thus have a preponderant role in determining the electrical and bonding properties of Ca_{1-x} Np_x Sn_3 substance. We anticipate that future theoretical and experimental research on this interesting material will be stimulated with the results of the present study.

(a) 

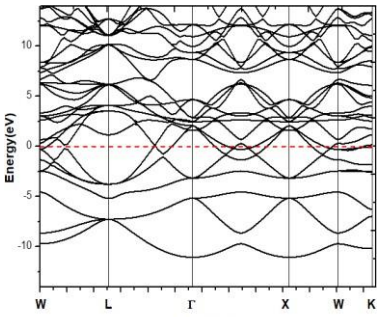
(b) 

Figure 1: crystal structure (a) , Calculated band structures (b) of Ca_{1-x} Np_x Sn_3 (x=0)

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INVESTIGATION OF TERNARY INTERMETALLIC HALF-HEUSLER COMPOUNDS *AIrSb (A= Hf, Ti)* WITH 18 VALENCE ELECTRONS: A THEORETICAL EXPLORATION

M. Hadbi[1,] , K. D*emmouche[2], H. Elarab[3], K. Chaoui[4]*

[1,2] Materials Science and Applications Laboratory. Faculty of Sciences and Technology. University of AinTemouchent Belhadj Bouchaib, B.P. 284. 46000. Algeria

[3] Laboratoire d'études physico-chimiques, Université Dr Moulay Tahar, Saida 20000, Algeria

[4]Laboratoire De Physique, Université 8 Mai 1945, BP 401, 24000 Guelma, Algeria

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** Corresponding author: mohammed.hadbi@univ-temouchent.edu.dz*

Keywords : Structural and Electronic Properties, Elastic Constants, Semiconductors, Half-Heusler Alloys, DFT, VASP.

Abstract :

This study delves into the structural, elastic, and electronic characteristics of ternary intermetallic Half-Heusler (HH) compounds AIrSb A= Hf, Ti), all of which possess 18 valence electrons. Employing the Vienna ab-initio Simulation Package (VASP) [1], we conducted a comprehensive theoretical analysis based on density functional theory (DFT) [2]. Specifically, we utilized the GGA-PBE approximation [3] for calculating exchange and correlation energies.

Our findings are meticulously compared to prior experimental and theoretical investigations. The investigated compounds exhibit crystalline structures within the cubic F4¯3 m space group (N°:216). Regarding structural properties, we computed the cell parameters, yielding results in close agreement with experimental data. Furthermore, our analysis confirms the mechanical stability of these compounds through the determination of the Tensor of elastic stiffness constants (Cij). In terms of electronic properties, our

research identifies these materials assemiconductors with an indirect band gap.

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PREDICTION OF THE STRUCTURE, ELECTRONIC, AND MAGNETIC PROPERTIES OF $CrMnCo_2Si_2$ DOUBLE HALF-HEUSLER ALLOYS

H. Elarabi[1], *F. Khelfaoui*[1], *K. Boudia*[2], *M. Hadbi*[3]

[1]*Laboratory of physicochemical studies, University of Saida-Dr. Moulay Tahar, Saida 20000, Algeria*

[2]*University of Tissemsilt, Ahmed Ben Yahia El-Wanchrissi, Algeria*

[3]*University of Ain Temouchent Belhadj Bouchaib, B.P. 284. 46000 Ain Temouchent. Algeria.*

** hiba.elarabi@univ-saida.dz*

Keywords : Half-metal, Heusler alloy, Spin-polarization, mechanical stability, FP-LAPW

Abstract :

The structural, electrical, and magnetic characteristics of CrCoSi and MnCoSi parent HH alloys, as well as their CrMnCo2Si2 daughter DHH compound, are investigated using the Wien2k code and the augmented plane waves technique (FP-LAPW). The stability of the CrCoSi and MnCoSi alloys' half Heusler structures has been tested for their non-magnetic and ferromagnetic phases, revealing that the latter phase of the type I arrangement is the most stable. The CrMnCo2Si2 DHH alloy is created and researched as a derivation of the discovered structural and magnetic ground states of CrCoSi and MnCoSiHH alloys. This DDH and its CrCoSi parent HH have been shown to be deformation resistant and may be categorized as ductile materials, while the MnCoSi compound is brittle. By the gradient generalized approximation (GGA).

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INVESTIGATION OF MECHANICAL PROPERTIES OF TMDS MATERIALS BY DFT

LOUAFI.Widad[1,] REZOUALI.Karim[1]*

[1]Laboratoire de Physique Théorique, Faculté des sciences exactes, Université de Bejaia, 06000 Bejaia, Algérie

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** widad.louafi@univ-bejaia.dz*

Keywords : heterostructures of vdW, Density Functional Theory, mechanical properties .

Abstract :

In this study, we conducted Density Functional Theory (DFT) calculations to analyze the structural and mechanical characteristics of heterostructures of vdW. The investigation of its electronic band structure revealed that, akin to fundamental constituents, the bilayers possesses adirect band gap, rendering it a delicate material. Transition metal dichalcogenides (TMDs) are a class of captivating substances, comprising atomically thin semiconductors with the formula MX2, where M signifies a transition metal atom (such as Mo or W) and X represents a chalcogen atom (S, Se, or Te). These materials exhibit small direct bandgaps, positioned within the visible and near-infrared spectrum [1,2], bestowing them with early allure due to their distinct physicochemical traits and potential applications in electronics and optoelectronics.WSe2, for instance, finds utility in field-effect transistors (FETs), logic circuit integration, and optoelectronic tools. To comprehensively fathom the properties of such materials, a blend of insightful first-principles investigations and experimental approaches proves indispensable. Accordingly, we propose an exploration of the structural and mechanical attributes of van der Waals heterostructures

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PHASE STABILITY, ELECTRONIC, MAGNETIC AND ELASTIC PROPERTIES OF Os2VGe HEUSLER COMPOUND.

Oussama Baraka [1, 2].

[1] *Laboratory of Study of Materials and Optical Instrumentations, Faculty of Exact Science, Djillali LiabesUniversity, Sidi Bel Abbes 22000, Algeria.*

[2] *Process Engineering Department, Faculty of Technology, Hassiba Benbouali University of Chlef, 02000, Algeria.*

b.oussama@univ-chlef.dz

Keywords : Heusler compound, FP-LAPW, magnetic properties, mBJ approach, half metallic.

Abstract :

The remarkable properties of the Heusler compounds and their applications in photovoltaics, optoelectronics, and spintronic devices [1, 2, 3] have attracted much scientific attention. In this study, we employ the FP-LAPW method [4] based on DFT [5], with the generalized gradient approximation (GGA-PBE) , and the modified Becke-Johnson potential (mBJ-GGA) for the exchange and correlation interaction in order to investigate the structural, electronic, magnetic, and elastic properties of the Os_2VGe Heusler compound.

For structural properties, it can be seen that the Cu_2MnAl-type structure is energetically more favorable than the Hg_2CuTi-type structure, the result reported here for the equilibrium lattice constant is in good agreement with the equilibrium lattice mentioned in the reference [4]. The Os_2VGe compound is energetically stable, according to the negative formation energy. The computed total magnetic moment is 0.995 μ_B with GGA and 1.000 μ_B with mBJ-GGA, it conforms with the Slater-Pauling rule, $M_T=Z_T$ -18, where Z_T is the number of valence electronsin Os_2VGe, the contribution of partially filled d-states of V atom generates this total moment. The result of the electronic structure shows a spin gapless semiconductor character with GGAand a half-metallic character with mBJ-GGA, the use of mBj had a considerable impact on the electronic (value of gap) properties of our compound. The elastic constants, C_{ij}, and other elastic moduli have been predicted, and our compound's mechanical stability has been proven.

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SYNTHESIS AND PHYSICO-CHEMICAL PROPERTIES OF COPPER NANOPARTICLES

W. Souici[*] S. Mahtout[1] A. Souici[2]

*1Laboratory of Theoretical Physics, Faculty of Exact Sciences, University of Bejaia, 06000 Bejaia Algeria*2*
*Laboratory of condensed physics, Faculty of Exact Sciences, University of Bejaia, 06000 Bejaia Algeria**

*3 Institut Lumière Matière, UMR5306 Université Lyon1-CNRS, Université de Lyon, 69622 villeurbanne Cedex,France**

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** Corresponding author: wafa.souici@univ-bejaia.dz*

Keywords : Copper nanoparticles, noble metals, stabilizing agent, synthesis.

Abstract :

Nanoparticles of noble metals have been the subject of numerous studies because of their specific properties and their prospects for use in different fields of application: catalysis, biology, and photonics [1-2]. Besides these applications, medical imaging based on the detection of luminescent photons, information storage, electrochemical detection and photothermy of cancer cells are now their potential fields of application [3]. In this work,we dedicated the synthesis of nanoparticles of noble metals in colloidal solution using chemical way; we reduced the copper sulfate solution (CuSO4×5H2O) by ascorbic acid with and without the presence of Gum Arabic (AG) in different concentrations as a stabilizing agent. The XRD analysis confirms the formation of copper nanoparticles and clearly shows the effect of AG molecule concentration on the final size of the nanoparticles.

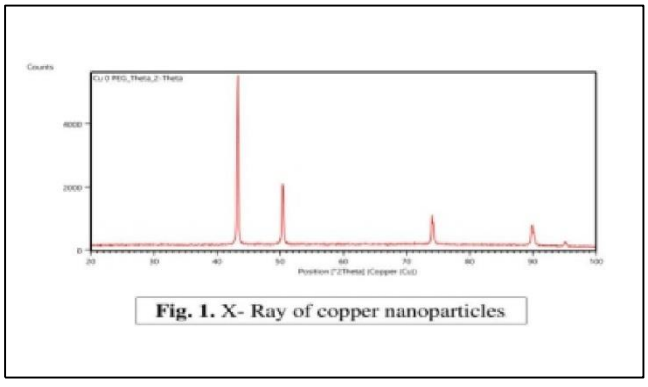

Fig. 1. X- Ray of copper nanoparticles

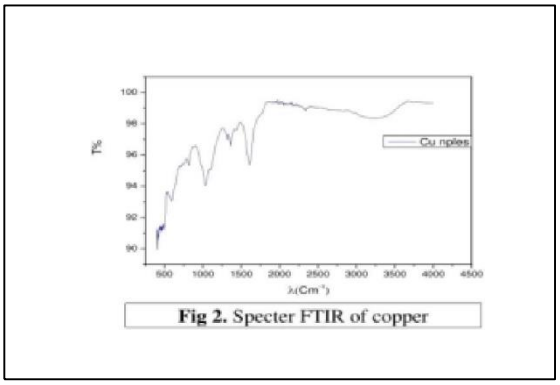

Fig 2. Specter FTIR of copper

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DEVELOPING ASPHALT CONCRETE PROPERTIES USING POLYMERS

Z.Bounaadja[1], L.Djimilli[1]*

[1] University of Annaba, Annaba, BP3029, Algeria

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** Corresponding author: zouzouboukouba@gmail.com*

Keywords : Polymer, Bitumen, Coated, Resistances.**Abstract :**

Summary. Polymer-modified bitumens have been used for several years to reduce the severity of deterioration and to prolong the useful life of hot mixes. To increase the performance of these binders, modification techniques are therefore used. The objective of the modification is to produce an "ideal" binder which should have improved cohesiveness and adhesiveness and a very low thermal susceptibility throughout the range of temperatures of use. Our research is a preliminary study for an experimental study later, this research collects theoretical data (the different types of polymers used for the modification of asphalts, compatibility of bitumens and polymers).

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THEORETICAL STUDY OF THE OPTICAL PROPERTIES OF $CdSnP_2$ CHALCOPYRITE

N.Taguida[1]✉, *S.Benlamari*[2], *H. Meradj*[2] and *S. Ghemid*[2]

[1] *LPCM Laboratory, Physics Department, Faculty of Matter Sciences, University of Chadli Bendjedid , El-Tarf*

[2] *LPR Laboratory, Physics Department, Faculty of Matter Sciences, University of Badji ,Mokhtar Annaba, Algeria*

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taguida-nesrine@univ-eltarf.dz

Keywords : WIEN2k, Chalcopyrite, DFT, Optical properties.

Abstract

The aim of this study is to calculate the optical properties of $CdSnP_2$ chalcopyrite materials that crystallizes in tetragonal structure, belonging to the $I\bar{4}2d$ (#122) space group The calculations are performed by the density functional theory (DFT) [1] implemented in Wien2k[2].

The exchange-correlation potential is treated by the local density approximation (LDA) and the generalized approximation PBE-GGA. The computed structural parameters for the studied compounds such as the equilibrium lattice constants, tetragonal distortion and bond lengthsare in good agreement with the experimental and theoretical data.

To understand the optical properties, the linear optical properties namely the real andimaginary parts of dielectric function, refractive index and extinction coefficientare calculatedover a wide range of energy, 0–30 eV.

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POSTER PRESENTATIONS

COMPARATIVE ANALYSIS OF PHYSICAL PROPERTIES OF Rh-BASED HEUSLERS: AB INITIO EXPLORATION

A. Bendris[*1] *S. Amari*[1,2]

[1]*Faculty of Nature and Life Science, HassibaBenbouali University of Chlef, 02000, Algeria.*

[2]*Laboratoire de Modélisation et Simulation en Sciences des Matériaux, Université DjillaliLiabès de Sidi Bel-Abbès, Sidi Bel-Abbès, 22000, Algérie.*

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** Corresponding author: benidris_ahmed@yahoo.fr*

Keywords : Ab-initio calculations, Electronic structure, elastic constants.

Abstract :

In this study, electronic and magnetic properties of twoHeusler alloysRh_2CoSn and Rh_2CoPb, were investigated using the full-potential linearized augmented plane-wave (FP-LAPW) method and the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) for the exchange-correlation energy and potential. The electronic structure in the ferromagnetic configuration shows metallic character. We also calculate the elastic constants, bulk modulus, shear modulus, and universal elastic anisotropy to study the mechanical stability.We used the gibbs code to calculate and predict some thermodynamic properties such as entropy, heat capacity, and phonon free energy of Rh2CoSn and Rh2CoPb alloys. We hope that our work can provide guidance for new spintronic materials and magnetic-intelligent materials among Heusler alloys.

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Welding of Dissimilar Materials.

Belkacem Tahir.

University Of Ouargla.

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Taher32bel@gmail.com

Keywords : Dissimilar welding, mechanical properties, solubility, friction welding

Abstract :

The welding of dissimilar materials is of great interest since it allows to innovate in the world of multi-materials by proposing new technological solutions in systems where strongly different properties may be required (weight gain and mechanical strength for example). Heterogeneous welding is applied in several industrial fields and in particular transport fields such as aeronautics, naval or automotive and also the petroleum industry.

However, the feasibility of such combinations is often limited by the large difference in the thermo- physical properties of materials and their chemical nature (solubility, formation of fragile phases, oxidation etc.) [1]. for this reason, several dissimilar metal welding processes have been innovated and are divided into two main categories. The first is based on melting at the contact joint like laser welding; and the second category is based on solid state welding like friction welding. On the other hand, the number of dissimilar metals welded in the petroleum industry until today remains very limited [2], hence the interest to contribute in this research axis. Therefore, the purpose of this research is to focus on welding dissimilar materials used in the petroleum industry.

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INVESTIGATION OF THE ELECTRONIC, ELASTIC, AND OPTICAL PROPERTIES OF Sc_2PbZ (Z=Si, Ge, Sn) HEUSLERCOMPOUNDS: FIRST-PRINCIPLES CALCULATIONS

G. Uğur[1,*], S. Er[1], E. Güler[2]

[1] Gazi University, Department of Physics, 06500 Ankara, TURKEY

[2] Ankara Hacı Bayram Veli University, Department of Physics, 06900 Ankara, TURKEY

** G. Uğur: gokay@gazi.edu.tr*

Keywords : Heusler compounds, density of states, elastic properties, dielectric function.

Abstract :

The electronic, elastic, and optical properties of Sc_2PbZ (Z=Si, Ge, Sn) Heusler compounds have been investigated in the GGA framework of density functional theory by employing the CASTEP code. The calculated electronic structures revealed that cubic Sc_2PbZ (Z=Si, Ge, Sn) compounds have metallic characteristics. All the studied Heusler compounds were found elastically stable from the elastic constant calculations. The calculated values of the Poisson ratio (ν) for Sc_2PbZ (Z=Si, Ge, Sn) are 0.33, 0.34, and 0.35, respectively, where these values indicate the metallic bonding characters of these compounds. Our presently computed elastic constants for Sc_2PbZ (Z=Si, Ge, Sn) alloys agree well with the former theoretical calculations[1]. The various optical properties, such as real and imaginary parts of the dielectric constant, optical conductivity, reflectivity, refractive index, and absorption coefficient, were also determined and discussed in detail.

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EXPLORING THE PHYSICAL, OPTOELECTRONIC AND MECHANICAL FEATURES OF A_2BCl_6 (A=Cs, Rb; B=Si, Ge, Sn) PEROVSKITES

G. Uğur[1,*], H.E. Gürel[1], E. Güler[2]

[1] Gazi University, Department of Physics, 06500 Ankara, TURKEY

[2] Ankara Hacı Bayram Veli University, Department of Physics, 06900 Ankara, TURKEY

** G. Uğur: gokay@gazi.edu.tr*

Keywords : Band gap, density of states, optical properties, perovskites.

Abstract :

The density functional theory was employed to explore the structural, electronic, optical, and mechanical features of A_2BCl_6 (A=Cs, Rb; B=Si, Ge, Sn) perovskites. The calculated band energy results disclose that all investigated perovskites are semiconductors. The mechanical stability of these materials was confirmed by the computed elastic constants within other mechanical parameters such as Young modulus, bulk modulus, shear modulus, Poisson's ratio, and Pugh's ratio. Further, several optical parameters, i.e., dielectric constant, refractive index, reflectivity, and optical conductivity, have also been investigated, and from the attained optical data, optoelectronic efficiency of A_2BCl_6 (A=Cs, Rb; B=Si, Ge, Sn)perovskites were discussed. Overall, presently obtained theoretical results are consistent with the earlier theoretical findings[1,2].

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THEORITICAL STUDY OF THE ELECTRONIC AND OPTICAL PROPERTIES OF NEW DOUBLE PEROVSKITE Ca_2CrIrO_6

Touaibia[1],* F.hemam [1]

[1]Applied and Theoretical Physics Laboratory (LPAT)Larbi tebessi university, Algeria

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** Corresponding author: ilham.touaibia@univ-tebessa.dz*

Keywords : DFT, half metal, absorption, optical conductivity.

Abstract :

The main objective of this study is to investigate the electronic and optical properties of Ca2CrIrO6 using the full potential linearized augmented plane wave (FPLAPW) method based on density functional theory. The results of the monoclinic phase predict an antiferromagnetic character. The densities of states results, obtained using the (GGA+U) approximation in this study, demonstrate the half-metallic behavior of Ca2CrIrO6. Optical properties of this material were studied through absorption and reflectivity, revealing a strong absorption peak at 200 × 10^4 cm-1 in the ultraviolet range. Based on the study's findings, Ca2CrIrO6 emerges as a strongcandidate for optoelectronic applications in the ultraviolet spectrum.

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CHARACTERIZATION OF XC48 STEEL'S SURFACE WITH SEM AND AFM WHILE STUDYING THE EFFECTIVENESS OF ORGANIC INHIBITORS AGAINST CORROSION WEAR IN HCL ACID OF XC48 STEEL'S SURFACE

I. Dakhouche[1,2], N. Khnnafi - Benghalem[1], N. Chafai[2].

[1]Emerging Materials Research Unit (URME), Institute of Optics and Precision Mechanics, University Ferhat Abbas-Setif 1.

[2]Laboratory of Electrochemistry of Molecular and Complex Materials (LEMMC), Department of Process Engineering, Faculty of Technology, University Ferhat Abbas Setif 1, 19000 Setif, Algeria.

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Email: ikramdakhouche.dr38@gmail.com

Keywords : Corrosion wear, Inhibitors, Protection, characterization of metallic alloys.

Abstract :

The corrosion wear of metals leads to many disasters and problems in industrial installations, and also causes environmental pollution, in particular the pollution of industrial waters by the metal oxides formed. From a chemical point of view, corrosion is an electrochemical reaction that occurs on the surface of a metal and leads to a modification of the mechanical, physicochemical and electromagnetic properties.

To avoid the aforementioned issues and to provide a long life for the metals used in industrial installations, corrosion protection must be addressed in this context. Generally, the solution chosen must be compliant with the guidelines for environmental protection and enable the recycling or elimination of the individual components upon completion of their useful lives. In order to protect metals from corrosion, a number of methods have been utilized. Among these, corrosion inhibitors have been described. It's fascinating how a corrosion inhibitor is applied. This kind of substance slows or stops the corrosion process of a metal when introduced in few doses to the corrosive medium.

Corrosion inhibitors made of organic compounds are now frequently employed to shield metals from rust in a variety of conditions. This work evaluates the corrosion inhibiting activity of two different organic inhibitors using the microscopic methods of characterization (SEM and AFM), which have been shown in our experimental studies to be very effective corrosion inhibitors against the corrosion wear of XC48 steel in acidic solution.

Ab initio study of structural, electronic, and optical properties of the $Cs_2AgBiCl_6$ halide double perovskite

Tahar. BELLAKHDAR[1,], Zakia. NABI [1], Badra. BOUABDALLAH[1]*

[1]Condensed matter and sustainable development Laboratory,Materials and Sustainable Development Department, Faculty of Science, University of Sidi-Bel-Abbes, Sidi-Bel-Abbes, 22000-Algeria.

* *taharbellakhdar@gmail.com*

Key words : Halide Double Perovskite; Optoelectronic propertie, ; FP-LAPW ; GGA-mbj.

Abstract :

In this work we have performed a theoretical study using the full potential linearized augmented plane wave approach (FP-LAPW), based on the theory of density functional theory (DFT)[1] implemented in the WIEN2K code[2], to determine the structural and Optoelectronic properties of double perovskite $Cs_2AgBiCl_6$.The exchange and correlation potential is treated by the generalized approximation (GGA)[3] and the modified approximation of Beck Jonhson (mBJ)[4] . The computed lattice constant was found to be in agreement with the available experimental and theoretical results. The electronic profile shows a semiconducting nature with an indirect band gap along the direction (X-Γ) with a small effective mass. The optical absorption coefficient has been determined showing a high-absorption (> 10^4 cm^{-1}) in the visible spectrum highly valued for solar cells and optoelectronics.

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AB-INITIO STUDY OF ELECTRONIC, OPTICAL, AND ELASTIC PROPERTIES OF CSPBI3 PEROVSKITE.

K.Chaoui[1],, N.E.A Doghmane[2], M.Hadbi[3], K.Zanat[1].*
[1] Laboratory of Guelma Physics, Faculty of Mathematics, Computer Science and MatterScience, University 8 Mai 1945, BP 401, 24000 Guelma, Algeria.
[2] Laboratory of Physique des Matériaux (L2PM), University of 8 Mai 1945, Guelma 24000, Algeria.
[3] Laboratory of Materials Science and Applications, Faculty of Sciences and Technology, University of Ain Temouchent Belhadj Bouchaib, B.P. 284. 46000 Ain Temouchent, Algeria.

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** Corresponding author: chaoui.khawla@univ-guelma.dz*

Keywords : Perovskite, ab-initio, photovoltaic applications.

Abstract :

The structural stability of the cubic perovskite CsPbI3, as well as its elastic, electronic, and optical properties, were calculated using the augmented wave approach incorporated within the Vienna ab-initio simulation package.Geometry optimization and electronic structure determination utilized the generalized gradient approximation (GGA) based on the Perdew– Burke–Ernzerhof (PBE) functional. The structural properties, such as the equilibrium lattice constant and bulk modulus along with its pressure-related derivative, are in good agreement with previous research. Electronic band structure and density of states calculations indicate that this substance possesses a direct band gap at the R symmetry point, measuring approximately 1.49eV under GGA and 1.81 eV under HSE06. Optical properties, including the real and imaginary parts of the dielectric function and absorption, were calculated in the energy range of [0–10 eV]. The results show that the optical absorption intensity reaches an order of 106 cm−1, which is considered excellent for photovoltaic applications.

CONTRIBUTION TO THE STUDY OF BINARY Al-X PHASE DIAGRAMS, PARTICULARITIES AND ADVANTAGES

F. Kali-Ali [1], S. Triaa[1], H. Khecha [1], S. Hamid Oudjana[1]*

[1] Laboratory of Materials Sciencs and Engineering, University of Sciences and Technology Houari Boumediene,(USTHB) PB 32 Al Alia 16111 Bab Ezzouar - Algiers - Algeria

** Corresponding author: fkaliali@usthb.dz*

Keywords : phase diagram,Al-X, phase transformation, data.

Abstract :

In this work, a detailed study is carried out on Al-X systems using their binary phase diagrams (1). Numerous information has been collected in these systems such as crystal structures and phase transformations. Forty eight Al-X systems were computed and all the data collected in order to make comparison sand then deduce the elements that present similar diagrams in relation to the information found. Results analysis show that the elements X = Ca, Sr and Ba - which are located on the same column (column II) of the periodic table - form the Al_4X compound with the same structure tI10 and that the elements X = V and Ta - which are on The same column (transition elements) - form the Al_3X compound with the same tI8 structure.

We can also notice that the rare earths x = La, Ce, Pr, Nd, Gd, Ho, Er, Yb, and U form all the compound of Al_2X formula with the structure Cf24.In addition, some of these rare earths have more one compound in common; we cite for example Nd and Pr that present five compounds in common with identical structures besides the Al_2X compound.

The results allow us to compute 21 systems with a defined congruent-compound transformation, 15 of which have temperatures above the melting temperature of the Al and X elements. It can also be noted that Al-X systems for X = Pt, Th and Y present two congruent points. The examination of the data reveals the presence of the AL_2X compound as a dominant congruent compound, 62% (of systems with congruent points) have congruent temperatures above the melting temperature of the two al and X elements.

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FIRST-PRINCIPLES STUDY OF THE HEUSLER SUPERCONDUCTOR Pd_2HfAl

M. Khatiri[1,], Y. Bourourou[1] and F. Faid[1]*

[1] Laboratoire des matériaux, applications et valorisation des énergies renouvelables (LMAVER), université AmarTelidji Laghouat, Algérie

** Corresponding author: mahdjoubakhatiri96@gmail.com*

Keywords : Pd_2HfAl, DFT, Heusler superconductors, Quantum Espresso.

Abstract :

In this work, a theoretical study was carried out on some physical properties of the Heusler compound Pd_2HfAl. The pseudo potential approach was used within the framework of density functional theory (DFT)[1] which is implemented in the Quantum Espresso[2] calculation code. The exchange and correlation potential were addressed by the generalized gradient approximation (GGA-PBE). The lattice parameter is in good agreement with the experimental and theoretical studies[3]. The electronic and vibrational properties indicate that our compound have a metallic nature and is dynamically stable. The superconducting critical temperature is calculated to be 3.7 K and the electron-phonon coupling parameter λ_{ep} of our full Heusler compound is 0.77.

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STRUCTURE AND CHARGE DELOCALIZATION OF THE PENTAVALENT HALOSILICONATES: THEORETICAL APPROACH

M.Aichi [1,3], M. Hafied.[2,3]

[1]Department matter sciences, Faculty of sciences and technology, University of Abbas Laghrour Khenchela,Algeria.

[2]Department of medicine, Faculty of medicine, University of Batna2, Algeria.

[3]Laboratory of materials and living chemistry activity-reactivity (LCMV-AR); University of Batna1-Algeria.

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Corresponding Autthor: aichimouhamed@yahoo.fr

Keywords: DFT, Pentavalent Halo-Siliconate, X-TMSOF, Charge Delocalization.

Abstract:

Structures of pentavalent halo-siliconate R-O-Si(CH3)3X- (X = F; Cl; Br) and (R = CH3; CH3-CH2-; -CH(CH3)2; -CH=CH2; -C6H5) are investigated using density functional theory (DFT) calculations at b3lyp-6-31G(d) level to understand the structure bonding characteristics and the delocalization of electronic density. Our results indicate that pentavalent fluoro-siliconate R-O-Si(CH3)3F- are stable intermediates for all substitutions with a trigonal bipyramidal geometry, the substituents prefer the axial position and the loss of alkoxy group is detected via the electronic charge transfer . In the case of X = Cl-;Br- intermediates adopt a structure in which the alkoxy group is nearly double bonding with silicon atom. The loss of Cl- and Br- detected by their negative charge (-0,941) and distance of (3,89) from the silicon center. Besides, the halotrimethylsilyloxyfurane (X-TMSOF) structures are also investigated at the same level of calculations. GIAO method permits to calculate δ29Si NMR shifts for the R-O-Si(CH3)3X- systems. A correlation between (Si–X) distance, Si-O-C angle and δ29Si NMR shifts has been drawn.

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EXAMINING THE IMPACT OF ANNEALING ON THE OPTICAL BAND GAP OF Dy-DOPED ZnO THIN FILMS FABRICATED VIA SPRAY PYROLYSIS AT DIFFERENT CONCENTRATIONS

M.Haroun[1],L.Bouhdjer[1] , S.Addala[1], H.Bareche[2]*

[1]*University ofAkliMohandOulhadjBouira,Bouira,Algeria.*

[2]*Department of Physics, University of M'sila,M'sila,Algeria.*

** Corresponding author: m.haroune@univ-bouira.dz*

Keywords : $(ZnO)_{1-x}(Dy)_x$ thin films,Uv-visble,Optical band gap.

Abstract :

Zinc oxide (ZnO) nanostructures exhibit an interesting wide optical bandgap, ranging from 3.10 to 3.37 eV. This property makes them one of the most popular semiconductors used in industrial applications (electronics, optoelectronics, etc). Naturally, like other intrinsic semiconductors, many studies have been conducted to explore their properties and adapt them to specific applications using various dopants. In recent decades, rare earth elements (Dy, Sm, Sn, etc.) used as dopants for ZnO thin films have displayed interesting optical and electrical properties [1,2].

The study had two main objectives: firstly, to produce Dy-doped ZnO thin films deposited on glass substratesusing the spray pyrolysis technique at varying concentrations, and secondly, to examine how the annealing process affects their optical band gap.To accomplish our objective, two characterization techniques were utilized: UV-visible spectroscopy and four-point probe measurements. The four-point probe was initially employed to assess the impact of Dy dopant concentration on resistivity and to determine the thickness of the resulting thin films. The UV-visible spectroscopy analysis was conductedto determine the optical band gap from the transmittance spectrum using the Taucplot method.

The samples underwent two annealing cycles with a time gap. The results showed that annealing had varying effects depending on the timing. The first process improved transmittance and widened the optical band gap, which can be explained by the enhanced crystallinity of the thin film. However, the second, under the same conditions, reduced transmittance and narrowed the band gap, could be attributed to crystalline degradation.

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THERMODYNAMIC REASSESSMENT OF THE ALUMINUM-GERMANIUM AND ALUMINUM-CERIUM SYSTEMS SUPPORTED BY FIRST-PRINCIPLES CALCULATIONS

R. Benhafid [1] and A. Belgacem Bouzida*

[1] Laboratory of Physical and Chemical studies of Materials (LEPCM),

Physics Department, Faculty of Matter Sciences, University of Batna 1, Batna, Algeria

Email : rabia.benhafid@univ-batna.dz

Keywords: Thermodynamic reassessment, phase diagrams, Gibbs energy, first principles calculations.

Abstract :

The present study reinvestigates the Al-M (M=Ce, Ge) phase diagrams and reoptimizes them thermodynamicly using the CALPHAD[1] method. The calculations are based on the determination of the Gibbs energy of the different phases of the system as a function of temperature and concentration.

The Gibbs free energies of the liquid, Fcc, and dimond phases in the Al-Ge systems were modeled by the substitutional solution model with the Redlich–Kister[2] formula. An agreement between the present calculated results and experimental data[3,4,5] was obtained. The phase diagram of Al-Ce system is reassesses by coupling the CALPHAD approach and Ab-initio calculations. The binary intermetallic compounds were treated as stoichiometric phases. There are the intermetallic compounds, some with two polymorphs. The total energies of five intermetallic compounds**:** α-$Al_{11}Ce_3$, Al_3Ce, Al_2Ce, AlCe and α-$AlCe_3$ were calculated by first-principles calculation using density functional theory approximation as implemented in the VASP[6] (Vienna Ab-initio Simulation Package) code and used in the CALPHAD approach to reassess the phase diagram. The Redlich-Kister polynomial model describes the liquid solution. A set of thermodynamic parameters were obtained for the Al-Ce system. The calculated phase diagram and thermodynamic properties are in good agreement with most of the accuracy available data.[7]

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THERMODYNAMIC CALCULATION OF PHASE EQUILIBRIA OF ERBIUM WITH BISMUTH AND TELLURIUM BINARY SYSTEMS

S. Bennoui[1], Y. Djaballah[1] and V. Vassieliev[2]*

[1] Laboratory of Physical and Chemical Studies of Materials (LEPCM), Physics Department, Faculty of Matter Sciences, University of Batna 1, Algeria

[2]Lomonosov Moscow State University, Chemistry Department, 119991 Moscow, Russia

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** Corresponding author: sonia.bennoui@univ-batna.dz*

Keyword : Calphad ; First-Principle calculations ; Bi-Er system ; Te-Er system.

Abstract :

A combination of the CALPHAD method and first-principles calculations was employed to evaluate the thermodynamic parameters of the Bi-Er and Te-Er systems. This approach was utilized to obtain new results and develop comprehensive thermodynamic descriptions for these systems[1]. In order to enhance the accuracy of the present optimization process, the first-principles method was employed to calculate the formation enthalpies at 0 K of Bi_2Er, BiEr, Bi_3Er_5, Te_3Er, Te_3Er_2, and TeEr. These calculations were conducted to supplement the available thermochemical property data[2]. In order to characterize the Gibbs free energy of the liquid phase in the Bi-Er and Te-Er systems, an associate model was employed. This model incorporated BiEr, TeEr, and Te_3Er_5 as the associated species composition.The binary intermetallic compounds were considered as stoichiometric phases[3]. Through this approach[4],a comprehensive and self-consistent set of thermodynamic parameters for the Bi-Er and Te-Er systems was obtained.

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AB-INITIO CALCULATIONS OF STRUCTURAL, MECANICAL, AND THERMODYNAMIC PROPERTIES OF AuM_2 COMPOUNDS (M= Na, K, Rb and Cs)

L. Bennour[1], Y. Djaballah[1], H. Righi[1] and D. Bahloul[2]*

[1] Laboratory of Physical and Chemical Study of Materials (LEPCM), Physics Department, Faculty of MatterScience, University of Batna 1, Algeria

[2]Higher National School of Renewable Energies, Environment and Sustainable DevelopmentFesdis, Batna 05078, Algeria.

** Corresponding author: linda.bennour@univ-batna.dz*

Keywords : Ab initio calculations, Gold-alkali intermetallics compounds, Structural and mechanical properties, Stability Phase.

Abstract

In this study, we report the ab-initio calculations for exploring the structural stability, mechanical, and thermodynamic properties of intermetallic compounds in the formula AuM_2 (M = Na, K, Rb, and Cs) in order to clarify their existence and stability in the alkali metal-gold binary systems Au-M at 0 K. Several suggested structures and suspect compounds, AuK_2 and $AuCs_2$, which were never reported, were also investigated. The obtained results indicate that the proposed compound $AuCs_2$ in the suggested structure $MoSi_2$ (*tI6*) is mechanically and dynamically stable but energetically stable close to 0 K. The compounds AuK_2 in Al_2Cu (*tI12*) and $AuRb_2$ in $MoSi_2$ (*tI6*) are energetically and mechanically stable but dynamically unstable in the considered structures, respectively. The elastic modulus and Debye temperature decrease with an increase in the lattice parameter throughout this series. The calculated Poisson's ratio values indicate that these compounds have an ionic character.

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ELABORATION AND CARACTERIZATION OF Cu/Ag/Mg COATINGS

Y.Bahloul. [1],* *, F.Lekmine*[2]

[1]*University Hadj Lakhdar, Batna 1, Laboratory of Physical and Chemical Studies of Materials (LEPCM)University Hadj Lakhdar, Batna 1 ,05000 Algeria*

[2]*University of Abbes Laghrour Khenchela, Physic Laboratory of Thin Films and Applications (LPCMA),University of Biskra, 07000 Algeria*

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** Corresponding author: bahloulyoucef1983@gmail.com*

Keywords : Morphology, structure, Cu-Ag-Mg coatings

Abstract :

To improve the effect of parameter s on the coating Cu-Ag-Mg, a wide variety of properties for coatings can be achieved by selecting different electrodeposition parameters. In this work, Cu-Ag-Mg coatings are deposited on copper substrates. X-ray diffraction (XRD), scanning electron microscope (SEM), energy dispersive spectroscopy (EDS) and microhardness analysis are used to study the effect of aditives on the morphology, phase structure, and microhardness of the coatings. The results confirm that the XRD patterns of the alloy deposits reveal that there are a number of sharp peaks in the images, indicating good crystallinity. The morphology of electrodeposited Cu-Ag-Mg coatings shows that the grains are spherical in nature for all samples, and EDS analysis of Cu-Ag-Mg composite confirms that the reduction of Cu decreases with increasing boric acid concentration. Moreover, reducing the concentration of boric acid in the Cu-Ag-Mg coating bath can lead to improved properties.

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METAL EFFECT ON THE PROPERTIES OF A GaN SCHOTTKY DIODE

N.E.I. Zaghoum[1],[*] N.E.A. Doghmane[2], S. Lakel[1] and Z. Hajoub[3]

[1] Laboratoire de matériaux semi-conducteurs et métalliques (LMSM), Université Mohamed Khider, Biskra 7000,Algérie.

[2] Laboratoire de physique des matériaux (L2PM), Université 8 mai 1945, Guelma 24000, Algérie.

[3]Laboratoire des Semi-Conducteurs, Département de Physique, Faculté des Sciences, Université Badji-Mokhtar, BP12, Annaba, DZ-23000, Algérie

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** Corresponding author: nourelimene.zeghoum@univ-biskra.dz*

Keywords: Schottky diode, GaN, metals, work function of metals

Abstract:

In recent years, a great deal of interest has been shown for large-gap semiconductors. They have become very attractive for high temperature, high frequency and high power applications. Among these semiconductors, GaN, with a gap of 3.39 eV at 300K, a critical field and a high saturation speed, seems to be the best choice for the realization of high voltage Schottky diodes. In this context, we investigate the metal effect on the characteristics of a GaN Schottky diode. Thus, the study of the influence of the metal work function on the diffusion voltage, the capacity of the structure and the width of the space charge zone led to several conclusions. The diffusion potential, V_d, which is an essential parameter of a Schottky diode controls the charge transport across the metal/semiconductor contact and determines the electrical behavior. In this study we quantified the relationship between the output workfunction of the metal, Φm, and this parameter through this relationship: $V_d = - \Phi m + 7.40$ (n type GaN) and $V_d = - \Phi m + 4.25$ (p type GaN). The capacity of the structure, C, whose the knowledge of its values leads to the determination of certain parameters such as the doping of GaN was also studied and important relationships were established: $C = - 0{,}25\Phi m + 1{,}85$ (n type GaN) and $C = - 2{,}5\Phi m + 10{,}8$ (p type GaN). As a final point, the width of the space charge zone, W, where several physical phenomena take place, plays an important role in determining the characteristics of the Schottky diode and particularly the capacitance of the structure. We have succeeded in establishing its variation law as a function of the output work of themetal considered. The form of the relationship strongly depends on the type of GaN. These results are of great importance in the design of GaN-based Schottky diodes for specific applications.

AB-INITIO CALCULATIONS OF THE PHYSICAL PROPERTIESOF 4D TRANSITION METAL ATOM DOPED SEMICONDUCTOR NANOSTRUCTURES

B. Siouani[1, 2], S. Safer[2], S. Mahtout[2]*

[1 1] Laboratory of Physical and Chemical studies of Materials ,

d'Alger 1, 16000 Alger, Algérie

[2] Laboratory of Theoric Physics, Faculty of Exactes Sciences, University of Bejaia, 06000 Bejaia, Algeria

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** Corresponding author: siouanichaouki@gmail.com*

Keywords : Ab-initio calculations, DFT, physical properties, semiconductor nanostructures.

Abstract :

We report herein the numerical analyses on the structural, electronic and magnetic properties of $PdAs_n$ (n= 0-20) clusters. A detailed study on the atomic composition dependent physical properties of these clusters has been performed employing spin polarized density functional theory (DFT) with the generalized gradient (GGA) approximation implemented in the SIESTA code. Structures, stabilities, electronic and magnetic properties are presented and discussed. Our theoretical investigation reveals that the transition metal atom Pd enhance the stability of pure arsenic clusters. The optimized clusters reveal that the most stable structures and their corresponding isomers have three dimensional configurations. The lowest energy structure of $PdAs_n$ generally differs from that of pure arsenic clusters. The relative stabilities have been studied in terms of the binding energies, fragmentation energies and second-order difference of energies for all $PdAs_n$ nanostructures. The binding energy per atom of doped arsenic clusters increases with the size n. The fragmentation energies show an oscillating behavior for all structures. The values of HOMO-LUMO gaps have a decreasing tendency along with the increasing number of As atoms in the cluster. The HOMO–LUMO gaps decrease considerably in our studied clusters which suggest an increase of metallic property. The total magnetic moment depends on the geometry, the position of Pd atom in the cluster, the charge transfer and orbital hybridization. The vertical ionization potential (VIP), vertical electronic affinity (VEA), chemical hardness (5), adiabatic electronic affinity (AEA) and adiabatic ionization potential (AIP) have also been investigated and discussed.

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STRUCTURAL , ELECTRONIC AND ELASTIC PROPERTIESOF $Zn_{1-x}Co_xSe$ AND $Zn_{1-x}Fe_xSe$ ALLOYS

F.Soltani[1], H. Baaziz[2], Z.Charifi[2]
[1]Physics Department, Faculty of Science, University of Batna 1, Algeria

[2] physics and chemistry of materials laboratory, University of M'sila, Algeria
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fatihasoltani2013@gmail.com

Keywords : the structural properties, zincblende , Semiconducting , half-metallic.

Abstract :

The structural, electronic, and elastic properties of $Zn_{1-x}Co_xSe$ and $Zn_{1-x}Fe_xSe$, ternary alloys are investigated at x = 0, 0.25 and 1 in the zincblende (B3) phase. The calculations are performed using all-electron full-potential linearised augmented plane-wave (FP-LAPW) [1] method within the framework of the density functional theory (DFT) [2] and the generalized gradient approximation (GGA) [3]. The electronic properties were performed using the modified Becke– Johnson potential combined with the GGA correlation (mBJ-GGA) [4] .The electronic structures are found to exhibit a semiconducting behaviour for $Zn_{1-x}Co_xSe$, ZnSe and a half-metallic behavior for $Zn_{1-x}Fe_xSe$ alloys at x = 0.25, while FeSe with x = 1.00 is found to exhibit a metallic behavior . In addition, we discuss the mechanical behaviour of binary and ternary compounds and all compounds studied here are mechanically stable.

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THERMODYNAMIC RE-ASSESSMENT OF THE SYSTEM (Bi-Li) SUPPORTED BY FIRST-PRINCIPLES CALCULATIONS.

F. Dziri [1], E. Belbacha [1], Y. Djaballah [1] and A. Belgacem Bouzida [1]*

[1] Laboratory of Physical and Chemical Studies of Materials (LEPCM),

University of Batna 1, 05000, Algeria

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** Corresponding author: email: fatima.dziri@univ-batna.dz*

Keywords : Ab-initio methods; CALPHAD; Enthalpy of formation; phase diagram.

Abstract :

The objective of this work was the thermodynamic modeling of the binary system Bi-Li, usingtwo complementary methods: the DFT method with ab-initio calculations and the CALPHAD approach (CALculation of PHase Diagrams) which has always been a very efficient tool fordetermining thermodynamic data and to establish phase diagrams.
The phase diagram of the Bi-Li system contains two defined compounds: BiLi and $BiLi_3$. Its enthalpy of formation is calculated using the Vasp (Vienna Ab-initio Simulation Package) code with the generalized gradient approximation as implemented by Perdewetal. (GGA-PBE) [2]. We have used also the local density approximation refined by Ceperley and Alder (LDA-CA) [3]. The CALPHAD evaluation of the Bi-Li system was then performed considering the calculated enthalpies of formation and the experimental phase equilibrium data. The liquid phasewas modeled by the Redlich-Kister [4] polynomial. The calculated phase diagram and thermodynamic properties agree well with the available experimental data.

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THERMODYNAMIC ASSESSMENT OF THE Ga–Pr SYSTEM SUPPORTED BY AB-INITIO CALCULATIONS

S.Boudraa, Y.Djaballah, A.Belgacem-Bouzida*

[1]*Laboratory of Physical and Chemical Studies of Materials (LEPCM), University of Batna1, Batna, Algeria.*

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**soumia.boudraa@univ-batna.dz*

Keywords : Thermodynamic assessment, ab-initio calculations, CALPHAD, Ga-Pr system.

Abstract :

Ab-initio calculations within density functional theory (DFT) with the projector augmented-wave technique (PAW)[1] were used to calculate the enthalpies of formation of the binary intermetallics in the Ga-Pr system. The thermodynamic data and the phase diagram of this system have been critically assessed according to the Calphad technique. The primary solid solutions in the Ga-Pr system were modeled with Redlich–Kister[2] polynomial.

The intermetallics compounds Ga_6Pr, Ga_2Pr, GaPr, Ga_3Pr_5 and $GaPr_2$ in addition to the suspected compound Ga_3Pr are taken into consideration in this optimization. The calculated enthalpies of formation using the VASP code[3,4] are used in the optimization of the Ga-Pr phase diagram which agrees well with the experimental data.

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MODELING OF THE Mg-Pb PHASE DIAGRAM BY COMBINING AB_INITIO CALCULATIONS WITH CALPHAD METHOD

R. Bouzida, Y. Djaballah, and A. Belgacem Bouzida

Laboratory of Physical and Chemical Studies of Materials (LEPCM), Physics Department, Faculty of Matter Sciences, University of Batna1, Algeria, 05000, Algeria.

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ramla.bouzida@univ-batna.dz

Keywords : First principles calculations, Mg-Pb system, Phase diagram.

Abstract :

First-principles calculations within density functional theory (DFT) with the projector augmented wave (PAW) [1] as implanted in the VASP code [2, 3] was used to investigate the stabilities of the binary intermetallics in the Mg-Pb system at 0 K. The intermetallic Mg_2Pb was investigated in its observed experimental structure. Enthalpy of formation of the Mg-Pb compounds has been calculated. In the second in a second stage we have optimized the Mg- Pb phase diagram using Calphad method. The calculated lattice constants, the enthalpies of formation and the assessed phase diagram are in good agreement with experimental and other theoretical results.

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THERMODYNAMIC MODELING OF THE Mg-Cu SYSTEM SUPPORTED BY AB-INITIO CALCULATIONS

I. Aggoun[1], F. Adjadj [1]

[1]Laboratory of Physical and Chemical Studies of Materials (LEPCM), Faculty of Matter Sciences, University of Batna1, Algeria

** Corresponding author: ilhem.aggoune@univ-batna.dz*

Keywords : Ab-initio, Mg-Cu system, VASP and BATNABIN code

Abstract :

The present study investigates the Mg-Cu binary system placing special emphasis on the two intermetallic compounds: Mg_2Cu and $MgCu_2$. We used ab-initio calculations to find the intermetallic stability of the intermetallic compounds of the Mg-Cu system. Our calculations are based on the functional density theory (DFT) implemented in the Vienna ab-initio simulation package (VASP) code.1 In the CALPHAD 2 optimization of this system, the study relies on the experimental phase diagram data and the enthalpies of formation of the compounds found by the ab initio calculations to estimate the phase diagram by BATNABIN code.

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CALCULATIONS OF THE STRUCTURAL, ELECTRONIC, OPTICAL, AND ELASTIC PARAMETERS OF CDSIX2 (X= P, AS) COMPOUNDS BASED ON FIRST-PRINCIPLES THEORY

H. Tiouiri [1,2], H. Baaziz [1,2], T. Ghellab[1,2] and Z. Charifi [1,2]*

[1]Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria

[2]Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria

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** Corresponding author: hadda.tiouiri@univ-msila.dz*

Keywords : Structural; Optical and elastic properties, Anisotropy, Mechanical stability.

Abstract :

We use density functional theory to study the structural, electronic, optical, and mechanical aspects of chalcopyrite's CdSiP2 and CdSiAs2, using both general gradient approximations and local density approximations. Replacing As with P significantly changed the lattice constant, elastic constant and dielectric properties. Our theoretical calculations are in good agreement with experimental data and other theoretical calculations. The electronic band structure analysis results indicate that all investigated compounds are semiconductors with energy bands directly at the Γ point. CdSiP2 has the highest elastic constant and bulk modulus, and CdSiAs2 has the highest shear modulus and elastic modulus values. In addition, special attention was paid to determining the direction-dependent linear compressibility and modulus of elasticity. In addition, special attention was paid to determining the direction-dependent linear compressibility and modulus of elasticity. In general, CdSiP2 and CdSiAs2 are isotropic, although their Young's modulus is anisotropic. In general, CdSiP2 and CdSiAs2 are isotropic, but their Young's modulus is anisotropic. Furthermore, the optical response of the compounds in the energy range from 0 eV to 14 eV was also investigated in terms of dielectric function, optical reflectance, refractive index, extinction coefficient, photoconductivity and electronic energy loss. Calculated optical results show that all compounds exhibit optical polarization anisotropy and are suitable for optoelectronic devices.

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RECENT INSIGHTS INTO ELECTRONIC PERFORMANCE AND MAGNETISM IN THE FE-SUBSTITUTED BASE: POSSIBLE CANDIDATES FOR MODERN SPINTRONICS DEVICES

N. Hamidane [1] , O. Hamidane.** [1],[1] University of Larbi Tebessi Tebessa, Algeria*

* nesrine_hamidane@yahoo.com

Keywords : DFT, FP-LAPW, $Ba_{1-x}Fe_xSe$, structural properties, DOS, BaSe

Abstract :

The fundamental properties of $Ba_{1-x}Fe_xSe$ ternary alloy are examined at concentration (0.25 and 0.50) 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 generalized gradient approximation of Wu and Cohen (GGA-WC).) 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 calculated structural parameters of BaSe are in good agreement with theoretical and experimental data. The electronic structures exhibit that the $Ba_{1-x}Fe_xSe$ materials for all concentrations are half-metallic ferromagnets with spin polarization of 100%.The exploration of the energy band gaps, however, revealed that these compounds have direct gaps at (Γ-Γ) direction of the spin up case. 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 4 μ_B per Fe atom respectively. Therefore, the $Ba_{0.75}Fe_{0.25}Se$ and $Ba_{0.50}Fe_{0.50}Se$ ternary alloy seems to be a new potential candidate for modern spintronics devices[3,4].

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INFLUENCE OF TITANIUM (TI) DOPING ON STRUCTURAL, ELECTRONIC, MAGNETIC, AND THERMODYNAMIC PROPERTIES OF BINARY CALCIUMCHALCOGENIDE SEMICONDUCTOR COMPOUNDS-A THEORETICAL INVESTIGATION USING DFT FUNCTIONAL.

O. Hamidane[1], N. Hamidane*[2]

1. University of Larbi Tebessi - Tebessa, Algeria. 2.University of Larbi Tebessi - Tebessa, Algeria.

* Corresponding author-mail : ouafa_hamidane@yahoo.com

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

Abstract

In this paper, we have investigated the structural, magnetic, electronic and thermodynamic propertiesof the cubic $Ca_{0.75}Ti_{0.25}Y$ (Y=S, Se, and Te) using density function theory (DFT) implemented in Wien2k code. The full-potential linearized augmented plane wave (FP-LAPW) method based on the generalized gradient approximation (GGA) was applied. The DMS semiconductor $Ca_{0.75}Ti_{0.25}Y$ (Y=S, Se, and Te) with cubic structure was more stable in the ferromagnetic configuration compared to the other phases. The electronic properties (band structure, electronic density of state) have a half-metallic (HM) behavior with 100% spin polarization at the Fermi level (E_F) for $Ca_{0.75}Ti_{0.25}S$, $Ca_{0.75}Ti_{0.25}Se$, and $Ca_{0.75}Ti_{0.25}Te$. This characteristic results from the metallic and semiconducting natures of majority- spin and minority-spin channels The magnetic moments calculated in $Ca_{0.75}Ti_{0.25}Y$ (Y=S, Se, and Te) were found to come specifically from Ti-3d electron states. The robustness of half-metallicity with changing the lattice parameters of $Ca_{0.75}Ti_{0.25}Y$ (Y=S, Se, and Te) alloys was discussed. Moreover, the thermodynamic properties announced in this work, seem to be important determinants for the synthesis of such materials.

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EXPERIMENTAL METHODS FOR THE CHARACTERIZATION OF AZO-METALLIC MATERIALS

S. Menassel[1], S. Chetioui[1,2],

[1]Technology Faculty, Université Mohamed Boudiaf, M'sila, Algérie.
[2]Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale-CHEMS-Faculté des Sciences exactes. Université des frères Mentouri-Constantine. Algérie.

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**E-mail: sihem.menassel@univ-msila.dz*

Keywords : characterization, experimental methods, metallic materials.

Abstract :

Azo compounds are very important in the fields of dyes, pigments and advanced materials. Azo dyes are synthetic colours that contain an azo group, as part of the structure. We are involved in the color generation mechanism of azo pigments typically characterized by the chromophore of the azo group (–N=N–). However, some types of azo pigments are also knownto possess the hydrazone structure (=N–NH–), often leading to the formation of intramolecular hydrogen bonds. The azo– hydrazone tautomerism in azo dyes has been known for more than a hundred years and is directly connected with the presence of at least one protic donor group in conjugation to the azo bridge (2-naphthol). In particular, azo dyes that contain a naphtholic hydroxyl group conjugated with the azo linkage exist in aqueous solution as an equilibrium mixture of two chemically distinct tautomers, the azo or hydrazone forms.

Recently, 1-phenylazo-2-naphthol derivatives have attracted attention because the phenylazo-naphtholate group can provide N,O-bidentate chelation to stabilize transition or main group metal complexes. Azo-metal chelates have also attracted increasing attention due to their interesting electronic and geometrical features in connection with their applications in molecular memory storage, non-linear optical elements and printing systems. Another advantage of complexes involving azo DNO's (dyes and pigments) and transition metal ions is the possibility to obtain new compounds with biological activity. Transition metals have also been used in the treatment of several diseases, as metal complexes which are capable of cleaving DNA under physiological conditions are of interest in the development of metal-based anticancer agents.This is an impetus for chemists to develop innovative strategies for the preparation of more effective, target-specific and preferably non-covalently bound anticancer drugs.

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THERMODYNAMIC ASSESSMENT OF THE In–Gd SYSTEM BY COMBINATION OF AB-INITIO CALCULATIONS AND CALPHAD APPROACH

Y.Mansouri[*1], A. Belgacem Bouzida, S. Boudraa, Y. Djaballah*

[1]*Laboratory of Physical and Chemical Studies of Materials (LEPCM), Physics Department, Faculty of Sciences Matter, University of Banta1, 05000,Algeria.*

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yakout.mansouri@univ-batna.dz

Keywords : In-Gd system, Ab-initio calculations, CALPHAD approach, Thermodynamic assessment .

Abstract :

In this work, the In-Gd binary system has been evaluated using the CALPHAD aproach[1]. First principles calculations within DFT (density functional theory)[2] were employed to calculate the enthalpies of formation of the intermetallic compounds of this system . The primary solid solution is described by the Redlich-Kister polynomial. The intermetallic compounds: InGd2, In_3Gd_5, InGd, In_5Gd_3 and In_3Gd are taken into consideration in this optimization and treated as stoichiometric. The values of the enthalpies of formation calculated by the VASP code are used in the optimization and finally to draw the In-Gd system phase diagram[3],which agrees well with the experimental data[4].

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AB-INITIO STUDY OF ELECTRONIC AND MAGNETIC PROPERTIES OF CoCrIrX COMPOUNDS (X= Ge, Sn, Si)

R .Beddiaf[1,2], H.Righi [2],Y.Djaballah[2] ,M. Diaf[2]*

[1] Higher National School of Renewable Energy, Environment & Sustainable Development Batna, Algeria

[2] Laboratory of Physical and Chemical Studies of Materials (LEPCM). Faculty of Matter Sciences , Department of Physics, University of Batna 1, Batna,

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** Corresponding author: raouf.beddiaf@hns-re2sd.dz*

Keywords : half Heusler, DFT, Electronic structure, Quantum-espresso

Abstract :

In this work, we present an ab-initio study of the structural, electronic, and magnetic properties of the Half-Heusler[1,2] quaternary compounds CoCrIrX (X = Ge, Sn, Si) using the Pseudo Potentials and Plane Waves method. This method is implemented in the QUANTUM ESPRESSO code and is based on Density Functional Theory (DFT). The exchange-correlation effect is treated using the Generalized Gradient Approximation (GGA-PBEsol). During this investigation, we conducted calculations of electronic state densities and energy band structures to predict the behavior of each of the mentioned compounds above.

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AB-INITIO CALCULATIONS AND THERMODYNAMIC MODELING OF SOME BASED RHENIUM BINARY SYSTEMS

H. Ghamri[1,] H. Righi[2]*

[1,2]Laboratory of Physical and chemical studies of materials (LEPCM)Physics, Department, Faculty of Matter Sciences, University of Batna1, Algeria

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** Corresponding author: houda.ghamri@univ-batna.dz*

Keywords : Calphadapproach, binary systems, first-principles calculations,phase diagram.

Abstract :

In the present work, combination of ab-initio calculation and Calphad approach was used for calculation of phase diagrams and thermodynamic functions for some based Rhenium systems.The enthalpies of formation of all intermediate compounds, at 0 K were predicted by first-principles method to supply the thermochemical data for these optimizations. The total energy of all binary compounds was calculated by means of VASP[1,2]with projector augmented wave (PAW) pseudopotentials[3] and the generalized gradient approximation (GGA)[4]using the high precision choice.

The solution phases were modelled with the sublattice formalism and the excess term of the Gibbs energy with the Redlich-Kister equation, while the intermetallic compounds which has a homogeneity range, were treated as the formula by a two-sublattice model. The rest of intermetallic phases were modeled as stoichiometric compounds. The calculated phase diagram obtained by using our first-principles resultsand the thermodynamic properties of the all systems are in satisfactory agreement with the experimental phase equilibriumdata.

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ELECTRONIC PROPERTIES OF Sb/As -DOPED MoSe2 MONOLAYER

B.Bradji[1], M L.Benkhedir[1]*

Echahid Cheikh Larbi Tebessi University, Tebessa, Algeria

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** Corresponding author: bouthaina.bradji@univ-tebessa.dz*

Keywords : Selenium dieselenide, Dichalcogenides, Two-dimensionalmaterial, Quantum Espresso.

Abstract :

Molebdenuim dieselenide $MoSe_2$ is a member of the family of monolayer transitions metals dichalcogenides (TMDCs), Which has recently gained considerable attention for various applications in electrochemical, Photocatalytic, And nano-optoelectronics (1).

Here we systematically study the effects of Sb and As wich are one of the group V element dopants on the electronic structure of a MoSe2 monolayer, The calculations were performed using the Quantum Espresso computational tool, Along with density functional theory (DFT) with ultra- soft pseudopotentials, the pseudopotentials are of the form of generalized-gradient approximation (GGA) developed by Perdew-Burke-Ernzerhof (PBE) (2), we used the 2H trigonal prismatic phase cause of their thermodynamic stability(3).

we calculate the electronic properties of pristine monolayer-MoSe2 and the doped MoSe2 with

the Sb then with As atoms, Where we can calculate the energy gap of this structures which

are in an ideal range for optoelectronic applications wich are always have a semiconductor with adirect band gap behavior,We then investigate the possibility of p-type doping in both doped structure, Then we determined the structural bands and density of states (DOS) and (PDOS) that helps us to explain the hybridization between orbitals and the changes resulting from doping.

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STRUCTURAL, ELASTIC, ELECTRONIC AND OPTICAL CHARACTERISTICS OF Ti_2CrZ (Z=Al, Ga, In, Si, Ge, Sn)HEUSLER ALLOYS

Ş. Uğur[1,], İ. Demirhan[1], M. Güler[2]*

[1] *Gazi University, Department of Physics, 06500 Ankara, TURKEY*

[2] *Ankara Hacı Bayram Veli University, Department of Physics, 06900 Ankara, TURKEY*

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* *Ş. Uğur: suleugur@gazi.edu.tr*

Keywords : Generalized gradient approximation, electronic band structures, elastic constants,optical properties.

Abstract :

The structural, electronic, elastic, and optical properties of cubic Ti_2CrZ (Z=Al, Ga, In, Si, Ge, Sn) alloys were investigated using density functional theory's generalized gradient approximation (GGA). Calculated band structure and density of states (DOS) have indicated that studied alloys have metallic behavior. Young's modulus values follow the Ti_2CrSi > Ti_2CrGe > Ti_2CrGa > Ti_2CrAl > Ti_2CrSn
> Ti_2CrIn order. Moreover, surveyed alloys show elastic stability and a ductile mechanical nature in their $L2_1$ crystal structure. The electronic and elastic results are compared with the available theoretical works[1].The optical properties, namely the dielectric function, absorption, refractivity, conductivity, and reflectivity, have also been calculated and evaluated.

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THROUGHPUT STUDY OF THE PHYSICAL PROPERTIES OF THE QUATERNARY HEUSLER ALLOYS TiZrRhX (X= Al, Ga)

B. M. Turki[1], H. Righi[2], M. Caid, D. Rached[1]*

[1] Djillali Liabès University of Sidi-Bel-Abbes, Faculty of Exact Sciences, Magnetic Materials Laboratory (LMM), Sidi-Bel-Abbès, 22000, Algeria

[2] Laboratory of Physical and Chemical Studies of Materials (LEPCM). Faculty of Matter Sciences of Batna 1

** Corresponding author: haroun.righi@univ-batna.dz*

Keywords : Quaternary Heusler alloys; magnetic materials

Abstract :

Through an ab-initio calculation employing the FP-LAPW method, we present detailed computational results of the physical peoperties of TiZrRhX (X= Al, Ga) quaternary Heusler alloys (QH's) based on a new atomic configuration. The equilibrium-ground-state of properties were predicted, revealing that the new investigated quaternary Heusler compounds are energetically stable in the α-phase structure within the ferromagnetic order. The present compounds' computed structural parameters are very similar to those obtained in theoretical data. Our compounds' formation energies have been examined to determine how thermodynamically stable they are. Both compounds exhibit a half-metallic ferromagnetic behavior with semiconductor character in the minority spin channel, as demonstrated by their magneto-electronic properties. This tendency is confirmed by the integer values of total magnetic moments, which likewise follow the Slater-Pauling rule. In order to evaluate the compounds' thermoelectric performance and predict potential high-tech applications, the transport properties are also calculated across a wide

temperature range, from 300 K to 800 K.

COMPUTATIONAL INVESTIGATION OF CO-BASED FULL HEUSLER ALLOY: STRUCTURAL, ELECTRONIC, ELASTICAND MAGNETIC PROPERTIES

S. Amara[1], S. Labidi[1], A. Amara[1], H. Kouarta[1]*

[1]Department of Physics, Faculty of sciences, Badji Mokhtar University, Annaba, Algeria

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*amara10seifeddine@gmail.com

Keywords: Co_2VGa, Heusler, Magnetic properties, Mechanical properties and Curie temperature.

Abstract :

We determined the structural, mechanical, electronic and magnetic properties of the Co2VGa by using full-potential linearized augmented plane-wave (FP-LAPW)[1,2] method simulation. The structural stability studies were performed for nonmagnetic, ferromagnetic and antiferromagnetic states. The elastic parameters and their derivatives have been calculated. The investigated energy band structure shows that the Co2VGa is half metallic. The total magnetic moments, stiffness constant of spin wave and the Curie temperature are also calculated. The magnetocaloric effect of this material are studied using the results obtained by FP-LAPW. The transition temperature, magnetic entropy change and relative cooling power are calculated.

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FILM THICKNESS EFFECT ON OPTICAL PROPERTIES OF TIN OXIDE (SnO_2) THIN FILMS GROWN VIA SOL-GEL METHODE

A.Youcef [1], A.Attaf [1],H. Saidi [1],O.Ben khetta [1]*

[1] Physics Laboratory of Thin Films and Applications LPCMA, University of Biskra, Algeria.

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** Corresponding author: aminaphysique9@gmail.com*

Keywords : tin oxide, thin films, sol gel, UV-Vis, optical band gap.

Abstract :

In this work, we investigated the effect of the thickness the various thicknesses (220-495-910 nm) on optical properties of SnO_2 thin films prepared by sol-gel (spin-coating) technique deposited onto glass substrates with speed (4000RPM) during the time of the deposition (30 sec). Was the preparation of the solution using a material of studied .stannous chloride ($SnCl_2.2H_2O$) as a basis and it was dissolved in appropriate amount of methanol (CH_3OH), the solution prepared at a concentration of 0.4M .The optical properties of tin dioxide have been investigated by ultraviolet visible spectroscopy in the range of wavelength (300-1000 nm), optical spectra show that these layers are transparent in the visible range, with average transmission from 70% to 80%. As well as the values measured of the optical band gap energy have increased with the increase in the thickness from 3.66eV at 3.77 eV

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FIRST-PRINCIPLES INVESTIGATIONS OF INTERMETALLICS IN THE DY-MN SYSTEM

F.Zerara [*] A. Belgacem-Bouzida, Y. Djaballah

[*] Laboratory of Physical and Chemical studies of Materials (LEPCM),

Physics Department, Faculty of Matter Sciences, University of Batna 1, Batna, Algeria

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** Corresponding author: fatima.zerara@univ-batna.dz*

Keywords : First principles calculations, VASP code, Dy-Mn alloy, phase stability.

Abstract :

The present study aims to investigate the stability of the different intermetallic compounds presented in the Dy-Mn system. At 0 K, It will be mainly focusing on the determination of the ground state line of this system. First-principles calculations within density functional theory (DFT) with the projector augmented wave (PAW)[1] as implemented in the Vienna ab-initio simulation package (VASP) code[2,3] were involved to calculate the formation energies of the pure elements and three intermetallic compounds: $DyMn_2$, Dy_6Mn_{23} and $DyMn_{12}$. The VASP code allows the optimization of the parameters a, b and c, using the generalized gradient approximation (GGA). Enthalpies of formation for the three previous intermetallicsfor the given binary phase diagram has been calculated. The obtained results shown that the calculated lattice constants and enthalpies of formation are in good agreement with experimental and other theoretical data.

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STUDY OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF INTERMETALLIC COMPOUNDS OF TYPEAB_2 FOR HYDROGEN STORAGE

S. AZIEZ [1,2], Y. Djaballah[2] and H. Righi[2]*

[1] *Center for Scientific and Technical research in physico-chimical analysis CRAPC, Indistrial Zone lelot n°30, Bou Ismail, Tipaza 42415, Algéria*

[2] *Laboratory of Physical and Chemical Studies of Materials (LEPCM), Physics Department, Faculty of MatterSciences, University of Batna 1, Algeria*

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* *aziez.siham@crapc.dz*

Keywords : Hydrogen storage, Intermetallic compounds.

Abstract :

In this work, we studied intermetallic compounds of type AB_2, which have attracted great attention for their significant hydrogen storage capacity, and use in different fields. The present study targets magnesium-based intermetallic using VASP code.

The aim of this VASP calculation is to examine the structural and electronic properties of$MgCu_2$ structure. These materials are interesting for their applications in the field of hydrogen storage. Various results obtained from the calculations will be presented and interpreted.

To determine the structural properties of the static equilibrium such as the structural parameter a_0, the Bulkmodulus B and its derivative, the total energy E_{tot} is calculated fordifferent values of the volume.

For the electronic properties of the compounds, the band structure gives the possible energies of an electron as a function of the wave vector. These bands are therefore represented inreciprocal space, and for simplicity, only the directions of highest symmetries in the first Brillouin zone are treated. The figure 1 of the $MgCu_2$, deduce overlapping of bands which appears at the Fermi level which confirms the metallic character of these materials. According to the total DOS presented in figure 2, it is a metallic state. Indeed, the Fermi level lies in themiddle of an allowed energy band, so since the peaks lie far from the Fermi energy proves that the compounds are not magnetic.

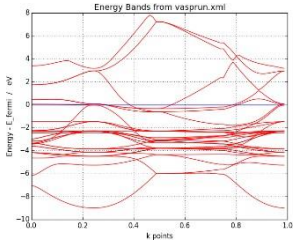

Figure 3: Band structure of MgCu2

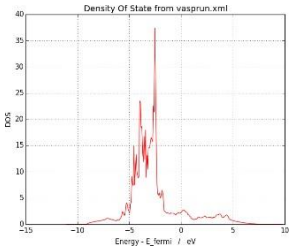

Figure 4: Total state density of $MgCu_2$.

MACHINE LEARNING ALGORITHMS IN PHASE DIAGRAMS

*Y. Tamerabet,[1, 2, *], F. Adjadj [1]*

[1] Laboratory of Physical and Chemical studies of Materials (LEPCM),

Physics Department, Faculty of Matter Sciences, University of Batna 1, Batna, Algeria

[2]National Higher School of Hydraulics, Blida

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** Corresponding author: y.tamerabet@ensh.dz*

Keywords: phase diagrams, long-short-term-memory (LSTM), gated recurrent unit (GRU).

Abstract :

The study of phase diagrams is difficult to implement experimentally. The use of modeling isa complementary method that can provide more information. A large number of significant works detailing deep learning approach and describing its various applications are available in the bibliography, but to the best of our knowledge, no work has been published that combines thermodynamics and phase diagrams with artificial intelligence approaches.
The aim of the present work is to provide the best neural network model to fit the experimental data with the least learning and validation error for plotting phase diagrams. Based on the model developed in our study, the results obtained are in line with the experimental results not only in terms of root-mean-square error but also in a very short execution time compared with other experimental methods. It would be interesting to test other deep learning methods and compare them with our LSTM and GRU models.

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THE ELECTRONIC STRUCTURE AND OPTIC PROPERTIES OF CS_2SNI_6 COMPOUND

T.Saadi [a, b *] *, Z. Charifi* [a, b, *], *H. Baaziz* [a, b]

[a] *Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria*

[b] *Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria*

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Corresponding author E-mail : *taieb.taieb0669@gmail.com*

Keywords : DFT, Structural properties, Energy gap, Density of states, dielectric function photovoltaic

Abstract

The structural, electronic and optical properties of Cs_2SnI_6 were studied using density function theory and the linearized augmented plane wave (FP-LAPW) method within the Wien2k code. LDA and GGA were used to treat the Exchange-Correlation (XC) potential.The results of the calculations showed that the studied compound is a semiconductor with a direct band gap Γ - Γ. The imaginary part of the dielectric function, the real part of the dielectric function, the refractive index, the extinction coefficient, the reflectance spectrum, the absorption coefficient, the optical conductivity and the energy loss function for Cs_2SnI_6 were also calculated. The electronic and optical properties have revealed that this compound is very useful for photovoltaic applications.

INSIGHTS INTO STRUCTURAL, ELECTRONIC ,MAGNETIC AND ELASTIC PROPERTIES OF Ru-BASED HEUSLER ALLOYS: PROBED BY DFT

S. Amari[1,*2] *A. Bendris*[1]

[1]*Faculty of Nature and Life Science, HassibaBenbouali University of Chlef, 02000, Algeria.*

[2]*Materials science modeling and simulation laboratory, Djillali-Liabes University, Sidi-Bel-Abbès, Algeria*

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** Corresponding author: siham_amari@yahoo.fr*

Key words : Ab initio calculations; FP-LAPW; Structural properties; Heusler alloys; elastic properties.

Abstract :

First-principles full-potential linearized augmented plane-wave method based on density functional theory is used to investigate the structural, electronic, magnetic and elastic properties of Ru based full-Heusler alloys Ru_2YSn (Y= Ni, Co). These full-Heusler alloys in different types structures: Cu_2MnAl and Hg_2CuTi were calculated within the generalized gradient approximation (GGA-PBE). The Cu2MnAl -type structure is found to be energetically more favorable than the Hg2CuTi-type .The ground state properties such as lattice constant, Bulk modulus local magnetic moment heat of formation have been calculated.The observed magnetism in these alloys is mainly from the 3d states of Ni and Co atoms.The elastic constants, Cij, and the other polycrystalline elastic moduli have been predicted and the mechanical stabilities of these alloys have been theoretically confirmed. To our knowledge the elasticconstants have not yet been measured or calculated, hence our results serve as a prediction for future study. Also, we presented results of the band structure and the density of states. The electronic structure in the ferromagnetic configuration shows metallic character.

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NUMERICAL CALCULATION OF AZO PHYSICALPROPERTIES FORTECHNOLOGICALAPPLICATIONS

N.E.A. Doghmane[1], K. Chaoui[2], M. Doghmane[1], S. Chettibi1*

[1] Material physics laboratory (L2PM), University ofMai 8, 1945, Guelma 24000, Algeria

[2] physics laboratory of Guelma (LPG), University ofMai 8, 1945, Guelma 24000, Algeria

** Corresponding author : doghmane.nozha@univ-guelma.dz*

Keywords : ZnO, Al-doping, Physical properties, photocatalysis.

Abstract :

In order to develop novel technological applications, a new approach based on low-cost, efficient andgood physical semiconductors properties is becoming a global priority and a very interesting field offundamental and applied research[1-3]. Thus, an alternative to well-known semiconductors, the zincoxide(ZnO) has recently been the subject of renewable research efforts due to its numerous advantages such asadequate band gap, photocatalytic mechanisms, high quantum efficiency, etc. Moreover, the doping ofthis material with aluminum (AZO) greatly improves its conduction and transparency in the visiblespectrum. In this context, for a phenomenon comprehension and property understanding, weinvestigatethe effects of aluminum doping on structural, electronic and optical properties of the most stable ZnOphase (hexagonal wurtzite). This study is curried out using DFT approximations via Wien2k simulationpackage. Theobtained results show that the fundamental band gap and the lattice parameters dependstrongly on Al doping. It is also shown that the introduction of Al into ZnO increases theabsorption edgeof the optical gap, confirming the results deduced experimentally and/or calculated theoretically.It shouldbe noted that the control of the band gap by doping opens up new device and integratedcircuit designs fornumerous applications in optoelectronics, energy and piezoelectricity.

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STRAIN EFFECTS ON STRUCTURAL, ELASTIC, ELECTRONIC, AND MAGNETIC PROPERTIES OFFEVYSB(Y=SC, Y) HEUSLERS COMPOUND

I. Bensehil[1,2] H. Baaziz[3,4],A. Kolli [2],Z. Charifi[3,4]*

[1] Faculty of Technology ,University of M'sila, B.P.166 , Ichbelia M'sila Algeria

[2]Laboratory of Surfaces and Interfaces Studies of Solid Materials,University of Setif 1, Algeria.

[3] Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria.

[4]Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria.

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** Corresponding author: ilhem.bensehil@univ-msila.dz*

Keywords : Quaternary Heusler compounds, Strain, Magnetic, Electronic

Abstract :

Since Groot's discovery of the first half metallic material, NiMnSb, in 1983, the scientific community hasbecome increasingly interested in the study of Heusler alloys[1]. Due to their unusual and interesting structural characteristics, magnetic properties, and many features, including metallic, insulating, semiconducting, half-metallic, and spin gapless semiconducting, these materials have garnered a lot of attention[2]. These materials are used for spintronics and magnetoelectronics applications such as spin filters, spininjection, magnetic tunnel junctions, giant magnetoresistance, spin transfer torque,memory devices, spin caloritronics, magnetic sensors, and neuromorphic and stochastic computing[3-5]

In this work, we have studied the structural, elastic, electronic and magnetic properties of FeVYSb(Y=Sc, Y) Heuslers compound basing on the density functional theory. The most stable structure has been found to be energetically favorable in face- centered cubic (FCC) structure with space group F43m, in which Fe,V, Y and Sb atoms are located at 4d, 4c, 4b and 4a Wyckoff positions, respectively. In the stable state, FeVScSb is ferromagnetic while FeVYSb is ferrimagnetic. The determined elastic constants (Cij) show that FeVYSb(Y=Sc, Y) is mechanically stable and ductile, and exhibit a notable elastic anisotropy. Electronic calculations indicate that FeVYSb(Y=Sc, Y) are semiconductors with band gap of 0.37 eV and
0.30 eV respectively. The total magnetic moment of these alloys is found to be equal to 3 μB which follows the Slater Pauling rule. The effect of uniform strain on electronic and magnetic properties is also studied, and the analysis show that FeVYSb (Y=Sc, Y) maintains its semi-conductivity in wide range of lattice parameter from 5.84 Å to 6.60 Å for FeVScSb, and from 6.11 Å to 6.70 Å for FeVYSb. The FeVYSb (Y= Sc,Y) Heuslers become half metal when the lattice parameter varies from 6.61 Å to 6.72 Å for FeVScSb and from 6.71 Å to 6.81 Å for FeVYSb. The magnetic moment remain equal to 3 μB under strain, which makes it hopeful in spintronic applications.

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THE ELECTRONIC STRUCTURE OF $XZRS_3$ COMPOUNDS (X = SR AND CA)

H. Ammi [a, b *] , *Z. Charifi* [b, c, *], *H. Baaziz* [b,]

[a,b]*Bouira university*

[b]*Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria*

[c] *Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria*

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** Corresponding author E-mail : hadjerimma1@gmail.com*

Keywords : DFT, Structural properties, Energy gap, Density of states, Perovskite compounds , photovoltaic

Abstract :

The study of the structural and electronic properties of $XZrS_3$ compounds (X = Sr and Ca) in the orthorhombic phase (Pnma) has been conducted and presented. Utilizing density functional theory (DFT) and Full-Potential Linearized Augmented Plane-Wave method (FP-LAPW), while considering the local density approximation (LDA) and generalized gradient approximation (GGA) for the exchange-correlation potential, along with the modified Tran and Blaha approach (mBJ) to compute energy band structures and density of states (DOS).The obtained crystal lattice parameters showed excellent agreement with experimental data. Our findings suggest that $CaZrS_3$ and $SrZrS_3$ compounds possess a crystalline structure similar to perovskite minerals, characterized by the general chemical formula ABX_3, where A and B are cations and X is an anion.Calculations of electronic band structures revealed that the studied compounds exhibit a direct band gap (Γ–Γ), classifying them as semiconductors. Moreover, we determined the energy gap values for $CaZrS_3$ and $SrZrS_3$ compounds, and compared them with other theoretical and experimental results.The results concerning the semiconducting nature and energy gap of the perovskite compounds, $CaZrS_3$ and $SrZrS_3$, underscore their significance both technologically and technically, with notable potential for significantly enhancing solar energy conversion efficiency in the photovoltaic field. This contributes to the advancement of renewable and sustainable energy technology.

CONTRIBUTION TO THE THERMODYNAMICSTUDY OF THE Al-Mg SYSTEM

*K.Bouzgou *, A. Abdessemed, Y. Djaballah*

[*] Laboratory of Physical and Chemical studies of Materials (LEPCM),

Physics Department, Faculty of Matter Sciences, University of Batna 1, Batna, Algeria

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** Corresponding author: khallaf.bouzgou@univ-batna.dz*

Keywords : Al-Mg system, ab-initio, CALPHAD, Batnabin.

Abstract :

The structural parameters and formation enthalpies of three compounds (Al_2Mg, $Al_{17}Mg_{12}$, Al_3Mg_2) are determined by ab-initio calculations with the generalized gradient approximation (GGA) as implemented in the VASP code. The structural parameters, are in agreement with the results obtained experimentally.

In second step a thermodynamic study of the system (Al-Mg) is carried out. We calculated the thermodynamic properties of this system and we established its phase diagram using two software programs: Batnabin and Pandat. The results obtained and the calculated phase diagram are in good agreement with the results of the literature.

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THERMODYNAMICS CONSTRUCTION AND SIGNIFICANCE OF CUPOURBAIX DIAGRAMS BASED AT 298 K (25 °C).

K. Oulmi[1],L.Lichani[1],N.Belkheiri[1],K.Chemcham[1]*

[1]Faculty of Matter Sciences. Department of chemistry, University of Batna1, Batna, Algeria

** Corresponding author:kafia.oulmi@univ-batna.dz*

Keywords : E-pH Diagram, Distribution diagram, Cu-H_2O, Cu-Gly-H_2O, Corrosion.

Abstract :

Pourbaix diagram and predominance area diagram are important thermodynamic stability diagrams. Various computer programs and tabulation software, such as Excel, Origin or Matlab have been used to facilitate the plot of these diagrams. These diagrams, besides elucidating the chemistry of the complexes involved in these systems, help to predict the optimum experimental conditions and the factors that affect the leaching processes, corrosion processes, electroplating, and the behavior of materials in various aqueous environments. To achieve the study's objectives, Simulations are carried out using an Excel spreadsheet to facilitate this process.

The E-pH diagrams for Metal-H_2O, Metal-Ligand-H_2O and distribution diagram of ligand species as function of pH systems are constructed using the equilibrium constant approach and the activity term method, relying on a comprehensive thermochemical database. This involves mathematical and computer-based calculations, illustrated through examples like the Cu-H_2O (Fig.1), Glycine-H_2O (fig.2) and Cu-Gly-H_2O systems. Comparatively, these diagrams offer a more comprehensive understanding of real hydrometallurgical processes and inhibitor corrosion when contrasted with traditional E-pH predominance diagrams. They help in understanding corrosion, electroplating, and the behavior of materials in various aqueous environments.

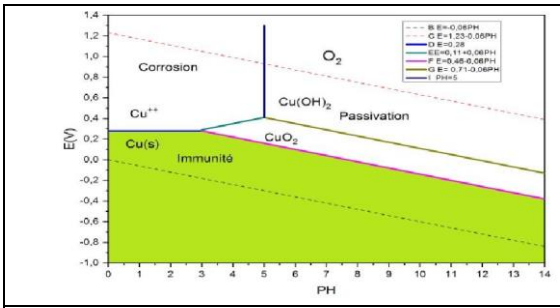

Fig.1: E-pH diagram for Cu(II)- water system at ($C=10^{-2}M$,P= 1atm andT=298 K).

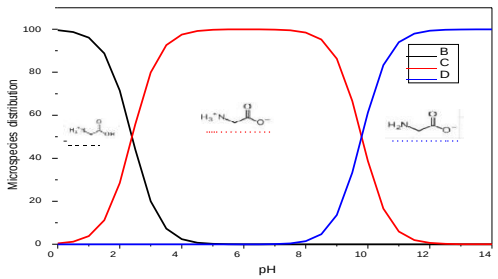

Fig.2: Dissociation profiles of glycine species as function of pH.

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CONSTRUCTION AND SIGNIFICANCE OF IRON POURBAIX DIAGRAMS BASED AT 298 K (25 °C).

K. Oulmi[1], D. Nezar[2],A.Lombarkia[1],A.Smaili[1]*

[1]*Faculty of Matter Sciences, Department of chemistry, University of Batna1, Batna, Algeria*

[2]*Faculty of Matter Sciences. Department of Physics, University of Batna1, Batna, Algeria*

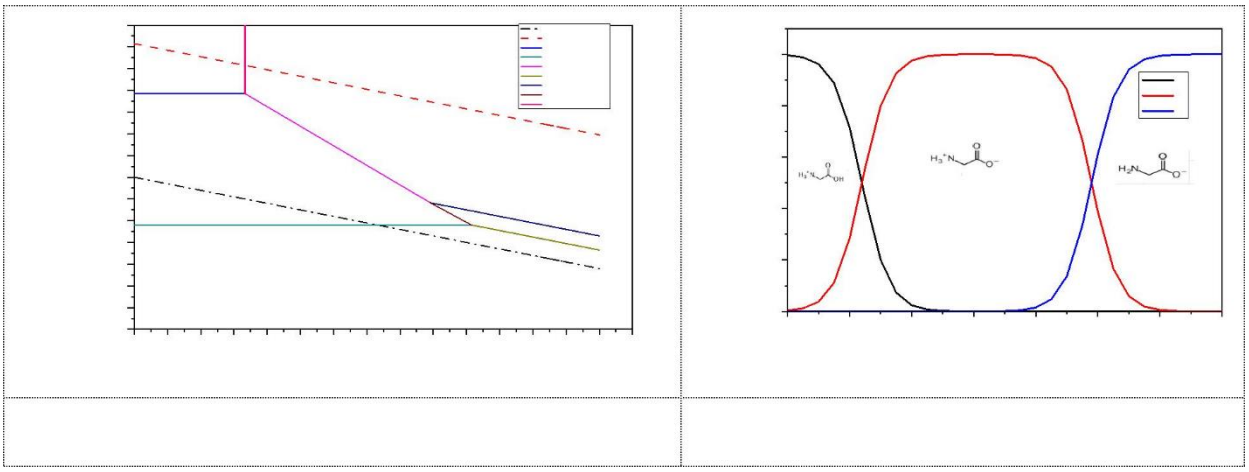
** Corresponding author : kafia.oulmi@univ-batna.dz*

Keywords : E-pH Diagram, Distribution diagram,Fe-H_2O, glycine-H_2O.

Abstract :

Pourbaix diagram and predominance area diagram are important thermodynamic stability diagrams. Various computer programs and tabulation software, such as Excel, Origin or Matlab have been used to facilitate the plot of these diagrams. These diagrams, besides elucidating the chemistry of the complexes involved in these systems, help to predict the optimum experimental conditions and the factors that affect the leaching processes, corrosion processes, electroplating, and the behavior of materials in various aqueous environments. To achieve the study's objectives, Simulations are carried out using an Excel spreadsheet to facilitate this process.

The equilibrium constant approach and activity term method are used to plot E-pH diagrams for Metal- H_20 and Metal-Ligand-H_20 systems based on the thermochemical database developed. The mathematical and computer calculation are described, with the Fe-H_20, Gly-H_20,Fe-Gly-H_20 systems as examples.More information on real hydrometallurgical processes can be obtained from these diagrams compared to conventional E-pH predominance diagrams. .



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OPTOELECTRONIC AND THERMOELECTRIC PROPERTIES OF BI2AL4SE8 COMPOUND: A DFT STUDY

*T. Ghellab[1,2] *. H. Baaziz[1,2], Z. Charifi[1,2].*

[1] Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria

[2] Laboratory of physics and chemistry of materials, University of M'sila Algeria

** torkia.ghellab@univ-msila.dz*

Keywords : Semiconductor, Grüneisen parameter, absorption coefficient, improving ZT.

Abstract :

Employing the FP-LAPW method, structural, electronic, optical, and thermoelectric parameters of $Bi_2Al_4Se_8$ compound are systematically investigated. The calculated structural parameters and axial ratio (*a*,*c*, *c/a*), as well as, atomic positions are found to be consistent with the experimental findings [1]. Using the mBJ-LDA approximation [2], band structure results reveal that $Bi_2Al_4Se_8$ is an indirect band gap semiconductor (E_g = 2.94 eV). One absorption peak of $\varepsilon_{2xx}(\omega)$ and $\varepsilon_{2zz}(\omega)$ at 3.66 eV and 3.77 eV energy level has been determined respectively. The dispersive part $\varepsilon_1(\omega)$ of the dielectric function shows a significant anisotropy. Consequently, $Bi_2Al_4Se_8$ can be utilized as a key component for optoelectronic devices since it exhibits a high absorption intensity. At room temperature, Grüneisen parameter of $Bi_2Al_4Se_8$ compound is found to be 1.045 corresponding to a calculated lattice thermal conductivity of 1.40 W/mK. The figure of merit *ZT* is found to increase as the temperature is elevated for both types of carriers. It attains maximum values of around 0.76 and 0.73 for *n* and *p*-type doping at -6.448×10^{18} /cm^3 and 4.635×10^{18} /cm^3, respectively. The values of S_{xx} Seebeck coefficient are found to be greater than those found in the S_{zz}. So, the transport along *xx*-axis is dominant. However, (σ_{zz}) is 79 % of (σ_{xx}) at high temperatures. The electronic thermal conductivity at high temperatures $(k_{e_{xx}})$ is larger. We found the value of $(k_{e_{zz}})$ to be 65% of that of $(k_{e_{xx}})$. At 900 K, ZT is 0.65, equivalent to a carrier concentration of $n_0 = 1.21891\times10^{21}$ cm^{-3}. The greater value of *ZT* is obviously 0.74 and this value is obtained by lowering the charge carrier concentration to $n_0 = 0.36582\times10^{21}$ cm^{-3}.

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AB-INITIO CALCULATIONS OF STRUCTURAL, ELECTRONIC AND ELASTICPROPERTIES OF $LiCu_2G$ HEUSLER COMPOUND

H. Bouheraoua *and E. Belbacha*

[1] *Laboratory of Physical and Chemical studies of Materials (LEPCM),*

Physics Department, Faculty of Matter Sciences, University of Batna 1, Batna, Algeria

** Email : habiba.bouheraoua@univ-batna.dz*

Keywords : DFT, Heusler alloy, GGA, WIEN2K, LiCu2Ga

Abstract :

Lithium alloys continue to be promising materials for anodes of chemical curent sources. So the search for new lithium – containing intermetallic phase and the study of their properties were the task of our study.

In this work , we presented a theoretical study on the structural, electronic and elestic properties of the heusler alloy LiCu2Ga. The purpose of the work is the investigation of physical parametres such us lattice constant, compressibility modulus, its derivative, state density, electronic band structure and elestic parameters. The calculation methode used is FP-LAPW which is incorporated into the WIEN2K code in the general framework of density functional theory (DFT). We use the generalized gradient density (GGA) approximation. The results obtained show that LiCu2Ga has a metallic character and is stable in the non-magnetic phase (NM).The elastic properties confirmed the mechanical stability of the compound.

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STRUCTURAL AND ELECTRONIC PROPERTIES OF SODIUM BASED FLUORO-PEROVSKITES "$NaMgF_3$" FROM FIRST-PRINCIPLE CALCULATION

R.Khenissa[*1] .A.Kerboub.E.Belbacha[1]*

[1] Laboratory of Physical and Chemical studies of Materials (LEPCM),

Physics Department, Faculty of Matter Sciences, University of Batna 1, Batna, Algeria

** Corresponding author: radhia.khenissa@univ-batna.dz*

Keywords: Fluoro-perovskite, DFT, pseudo-potentials, planeswaves, properties electronic

Abstract:

We have performed first principle calculation within the density functional theory (DFT) and the pseudo potentials with planes waves approach, for structural and electronic properties of the cubic Fluoro-perovskite "$NaMgF_3$". Using the CASTEP package[1] the calculations where performed within the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE) for exchange correlation energy[2].

The results show that both compounds are stable in the cubic Pm3m structure[3].

The electronic band structure calculations and bonding properties show that fluoro-perovskites have an indirect energy band gap (M–Γ) with a dominated ionic character.

Our results are in good agreement with the available experimental and theoretical results.

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MORPHOLOGY, PHASE STRUCTURE ANDMECHANICAL PROPERTIES OF Ni-Fe COATING

I.Zidani [1,], F.Lekmine[2]*

[1]University Hadj Lakhdar, Batna 1, Laboratory of Physical and Chemical Studies of Materials (LEPCM) Algeria
[2] University of Abbes Laghrour Khenchela, Physic Laboratory of Thin Films and Applications (LPCMA), University of Biskra, 07000 Algeria

** Corresponding author: ibtissem.zidani@univ-batna.dz*

Keywords : Morphology, Phase structure, Ni-Fe, Boric acid

Abstract :

To improve the properties of Ni-Fe coating, a wide variety of properties for coatings can be achieved by selecting different electrodeposition parameters. In this work, Ni-Fe coatings are deposited on copper substrates. X-ray diffraction (XRD), scanning electron microscope (SEM), energy dispersive spectroscopy (EDS) and microhardness analysis are used to study the effect of boric acid on the morphology, phase structure, nickel content and microhardness of the coatings. The results confirm that the XRD patterns of the alloy deposits reveal that there are a number of sharp peaks in the images, indicating good crystallinity. The morphology of electrodeposited Ni-Fe coatings shows that the grainsare spherical in nature for all samples, and EDS analysis of Ni-Fe composite confirms that the reductionof Ni decreases with increasing boric acid concentration. Moreover, reducing the concentration of boric acid in the Ni-Fe coating bath can lead to improved properties.

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THERMODYNAMIC MODELISATIONS AND OPTIMISATION OF THE Ca-Ga SYSTEM

H. Badi[1], R. Benhafid and A. Belgacem Bouzida*
[1] Laboratory of Physical and Chemical studies of Materials (LEPCM), Physics Department, Faculty of Matter Sciences, University of Batna 1, Batna, Algeria
Email : halima.badi@univ-batna.dz

Keywords: Thermodynamic modelisation, CALPHAD, Ca-Ga system, phase diagrams, excess energy.

Abstract :

The phase diagrams of the Ca-Ga binary system was established by Bruzzone[1]. The most recent information on this binary phase diagram was taken from the phase diagram compiled by Massalski.[2]

The main goal of our work is to restore the phase diagram of the Ca-Ga system using the CALPHAD[3] (Calculation of Phase Diagrams) approach. The binary excess energy terms are described using Redlich–Kister[4] polynomial model. The enthalpies of formation of the compounds of this system were taken from the literature, and evaluated and treated as stoichiometric compounds. The BATNABIN[5] code permits the modelization and the thermodynamic optimization of all phases of the Ca-Ga system. The PANDAT code permits to draw the phase diagram of this diagram using a TDB file.The results obtained as the equilibrium phase diagram of Ca-Ga system was compared with the experimental data[6,7]. A good agreement between the calculated results and experimental data was obtained.

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THERMODYNAMIC DESCRIPTION OF THE Ag–Hg AND Ag–Eu BINARY SYSTEMS

I. Ameziane [1], A. Belgacem Bouzida , A.Hidoussi, Y. Djaballah

[1] *Laboratory of Physical and Chemical Studies of Materials (LEPCM), Department of Physics, Faculty of Material Sciences, University of Batna 1, Batna, Algeria*

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Email:imane.ameziane@univ-batna.dz

Keywords : Phase diagram , CALPHAD method , Thermocalc, sublattice model

Abstract

The Ag–Hg and Ag-Eu binary systems were evaluated using the CALPHAD method through ThermoCalc software package[1]; the thermodynamic parameters involved in the Gibbs free energymodels of the phases are optimized based on all available literature experimental data including the phase equilibria information and few thermodynamic properties . The Gibbs free energies of the solution phases including liquid, fcc_A1 and The hcp_A3 were formulated with Redlich– Kister polynomial functions. The γ(Ag11 Hg15) phase in the Ag-Hg system and Ag_2Eu in the Ag-Eu system are described using sublattice model[2] because they have a homogeneity range and those of the intermetallic compounds Ag_5Eu, Ag_4Eu , AgEu , and Ag_2Eu_3 were treated as stoichiometric phases. As a result, two self-consistent thermodynamic data sets for describing theAg–Hg and Ag–Eu binary systems have been derived, and the calculated results show a satisfactory agreement with the corresponding experimental data reported in the literature.

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THERMODYNAMIC ASSESMENT OF THE Fe–Pb–Sb SYSTEM

A. Miloudi, F. Adjadj*

Laboratory of Physical and chemical studies of materials (LEPCM),

Physics Department, Faculty of Matter Sciences, University of Batna 1, Algeria

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** Corresponding author: anhar.miloudi@univ-batna.dz*

Keywords : Phase diagram, Fe-Sb-Pb system, Thermocalc, CALPHAD.

Abstract:

The Fe-Sb-Pb system is evaluated by CALPHAD method. The work consists in calculating the free enthalpies relating to the binary iron-antimony alloys on the basis of thermodynamic data noted in the bibliography [1].

The Fe-Sb-Pb system is investigated using PARROT module of the Thermocalc program created by Sundman et al[2].the Redlich-Kister equation [3] was used to model the solution phases.All binary intermetallic compoinds are cinsidered stoichiometric.

The estimated isothermal section of the ternary system Fe–Sb–Pb at 500 K correspond well with the experimental results. No ternary compounds were found in there section. There are three-phase regions, five two-phase regions and five single-phase regions in Fe–Pb–Sb system at 500 K.

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STRUCTURAL, ELECTRONIC, OPTICAL AND THERMOELECTRIC PROPERTIES OF PEROVESKITEALLOY $KMgH_3$

L. Amrani [1,] D. Bensaid[1,3] H .Rached[1]*

[1] Magnetic Materials Laboratory, Science Exact FacultyDjillali Liabes University of Sidi Bel Abbes, Algeria

[2]faculty of science and technology, BelHadj Bouchaib University, Ain Temouchent

[3]Electrical Engineering Faculty, Djillali Liabes University of Sidi Bel Abbes, Algeria

Keywords: Perovskite, FP-LAPW, DFT, GGA, HSE06, WIEN2K, BoltzTraP, Seebeck coefficient.

Abstract :

In this research, we conducted an investigation into the structural, electronic, optical, and thermoelectric characteristics of the Perovskite alloy $KMgH_3$. To anticipate these diverse properties, we applied simulation techniques utilizing the full-potential linearized augmented plane wave (FP-LAPW) method, which relies on Density Functional Theory (DFT) employing the Generalized Gradient Approximation (GGA) as proposed by Perdew-Burke- Ernzerhof [1]. Additionally, we employed the hybrid function (HSE06) to address the exchange and correlation term. This computational method is implemented within the WIEN2K software package [2]. This platform allowed us to determine the structural parameters at equilibrium. Electronic properties are also discussed, from the calculation of theelectronic band structure for all alloys in the most stable phase, our material exhibits semiconductor behavior with a direct gap of 1.130 eV. The use of the approximation (HSE06)as a correction of the terms of exchange and correlation allowed us to obtain a considerable improvement in the energy gap with a value of Eg=1.916 eV. In the optical part, we performed the calculation for reflectivity and refractive index. Also, we ended with thermoelectric properties using the BoltzTraP code [3] by calculating the Seebeck coefficient and thermoelectric power factor.

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DFT INVESTIGATIONS ON ELECTRONIC STRUCTURE, MECHANICAL STABILITY, AND MAGNETISM IN THE TERNARY FULL-HEUSLER ALLOYS Pd_2ZrZ (Z = Ga, Al)

B. Benichou[1,2,], H. Bouchenafa[3], Z. Nabi[2], B. Bouabdallah[2]*

[1] Department of Electronics, Faculty of Technology, Hassiba Benbouali University of Chlef, Chlef 02000,Algeria

[2] Computational Materials Physics Laboratory (CMPL), Faculty of Exact Sciences, Djillali Liabès University of Sidi Bel Abbès, Sidi Bel Abbès 22000, Algeria

[3] Laboratory for Theoretical Physics and Material Physics, Faculty of Exact Sciences and Informatics, Hassiba Benbouali University of Chlef, 02000 Chlef, Algeria

** Corresponding author: boucif_benichou@yahoo.fr*

Keywords: Structural properties, Pd-based full-Heusler alloys, FP-LAPW method, metal.

Abstract :

The electronic structure and magnetic moments of two Pd-based Heusler alloys, Pd_2ZrZ, with Z = Ga and Al, have been calculated via the *ab initio* spin-polarized full-potential linearized augmented plane-wave (FP-LAPW) method based on density functional theory and compared with other experimental and theoretical results. The exchange-correlation is handled using the generalized gradient approximation (GGA). It is found that these alloys are metallic ferromagnetic, and their structural parameters and magnetic moments are in good agreement with the experimental and theoreticalresults.[1,2,3,4] We also compute ground-state values, including elastic constants, shear moduli, Young's modulus, bulk modulus, and Poisson's ratio, which indicate that the compounds under study are mechanically stable, ductile, and anisotropic. Moreover, to the best of our knowledge, our work is the first to attempt to determine the elastic and mechanical properties of Pd_2ZrGa and Pd_2ZrAl compounds.

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CHARACTERIZATION OF THE THERMAL CONDUCTIVITY OF BULK MATERIALS AND THIN LAYERS BY AN EXPERIMENTAL METHOD CALLED “3 OMEGA”

A.A. Guermoudi[1,2,], P-Y. Cresson[3], A. Ouldabbas[4], T. Lasri[3]*

[1] *Hassiba Benbouali University of Chlef, Chlef, Algeria.*

[2] *Renewable Materials and Energies Research Unit (URMER) / Aboubekr Belkaid University of Tlemcen, Tlemcen, Algeria.*

[3] *Institute of Electronics, Microelectronics and Nanotechnology (IEMN) / Univ. Lille CNRS, Centrale Lille, ISEN, Univ. Valenciennes, Lille, France.*

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* *a.guermoudi@univ-chlef.dz*

Key words : 3-omega method, thin layers, heat source, thermal wave, temperature, thermal conductivity**.**

Abstract :

The objective of this work is to propose a way to measure thermal conductivity at room temperature. In this communication, we first describe the so-called 3-omega method which was introduced by D.G Cahill [1,2], then we present the results obtained during the characterization of a polymer material in a thin layer of 127 µm thick. This technique has been widely exploited to determine the thermal conductivity of a wide range of materials [3]. Due to its precision and low sensitivity to heat loss by radiation. The process uses a thin-film metal line (produced by an optical photolithography technique) which serves simultaneously to thermally disrupt the system and measure temperature variations of the sample. The temperature variation in the line is measured experimentally by detecting the third harmonic of the voltage which is proportional to the temperature variation [4,5]. This voltage carries the information allowing the value of the thermal conductivity of the material under test to be extracted..

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DENSITY FUNCTIONAL THEORY-BASED TIGHT BINDING METHOD (DFTB) STUDY: INVESTIGATION OF THE INFLUENCE OF HELICAL BN ORIENTATION ON THE ELECTRONIC PROPERTIES OF BNC-NANOTUBES

A. Khemissi[1], H. Khalfoun[2]*
[1,2] Laboratory for Theoretical Physics and Material Physics (LPTPM),
Faculty of Exact Sciences and Informatics,
HassibaBenbouali University, Chlef, Algeria

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** Corresponding author: a.khemissi@univ-chlef.dz*

Keywords : Boron Nitride Carbon nanotubes, electronic transport properties, band structurecalculations, wave functions.

Abstract :

Carbon nanotubes are cylindrical nanostructures composed of carbon atoms. They are one of the most widely studied and versatile nanomaterials. CNTs can be single-walled or multi-walled, with unique electronicproperties. They exhibit exceptional strength, electrical conductivity in various applications, from nanoelectronics to composite materials[1]. On the other hand, Boron Nitride Nanotubes are structural analogs of carbon nanotubes, but they consist of boron and nitrogen atoms instead of carbon. BNNTshave a seamless cylindrical structure and exhibit exceptional properties like electrical insulating properties. The BNC nanotubes are hybrid nanotubes that combine both boron nitride and carbon in their structure. They can have alternating boron nitride and carbon layers or have a mixed arrangement of boron nitride and carbon atoms within the same nanotube. BNC nanotubes inherit the properties of both CNTs and BNNTs, making them versatile materials with a wide range of potential applications. Their properties can be tuned by adjusting the position, orientation of boron nitride within the pristine carbon nanotube, offering control over electrical conductivity.

Using the density functional theory (DFT) based on the tight-binding method (TB), we have investigated the electronic properties and energetic stability for different arrangements and orientations of the helical zigzag boron nitride (BN) lines within the host armchair carbon heteronanotube. Our findings reveal that the semi-conducting properties remain consistent regardless of the orientation of BN atoms. Moreover, the nature of wave functions demonstrates propagating waves in the carbon segments, contingent upon the atoms interfaces. All calculations were performed using the DFTB+ software package[2].

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SITE PREFERENCE, ELECTRONIC STRUCTURE AND MECHANICAL PROPERTIES OF TERNARY ALLOYING ADDITIONS IN B2 Dy-Cu ALLOYS: FIRST-PRINCIPLES CALCULATIONS

A.Sekkal[1], N. Ben heroual[2], M. Sahlaoui[3], A. Ferouani[3]*

[1] National higher school of advanced technology (ENSTA) , 16001 Algeria

[2] Materials study and Prediction division DEPM-URMER, University of Abou Bekr Belkaid, Tlemcen, 13000 Algeria.

[3]higher school of applied Sciences , Tlemcen, Algeria

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** Corresponding author: asekkal.ph@gmail.com*

Keywords : DyCu compound, site preference, effect of alloying on electronic and mechanical properties, Ab initio calculations.

Abstract :

Binary rare-earth intermetallic compounds are attractive material from both fundamental and industrial perspectives and have a wide range of applications in engineering systems. In 2003, K. Gschneidner reported on the discovery of a number of ductile rare earth intermetallic compounds with the CsCl type-B2 structure. They are characterized by high melting point, high specific strength, good ductility, and excellent corrosion resistance [1-4]. The most recent interest in them is due to their high ductility and high fracture toughness at room temperature, as well as chemical stability. In this work, we propose to study the structural, electronic and mechanical properties of DyCu intermetallics which crystallize in the B2-CsCl type structure using the pseudo-potential method based on the density functional theory (DFT).) implemented in the VASP code. We also report the influence of substituted transition metals (V, Ni and Ti) on the crystallographic sites Y and Cu in order to understand their effects on the structural, electronic and mechanical properties of DyCu alloys. The analysis of densities of states and mechanical properties indicate that ternary alloys are more ductile compared to their parent binary compounds.

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THEORETICAL STUDY OF ELECTRONIC AND MAGNETIC PROPERTIES OFHALF-METAL Co_2MnGe

A. Bouhanna[1] , O. Zeggai[2,3], H . Bouhani-Benziane[4]

[1] Laboratory for Theoretical Physics and Material Physics, Department of Physics, Faculty of Exact Sciences and Informatics,Hassiba Benbouali University of Chlef, Chlef, Algeria

[2] Department of Common Core, Faculty of Exact Sciences and Informatics, Hassiba Ben Bouali University, BP 151,Chlef 02000, Algeria

[3]Research Unit Materials and Renewable Energy (URMER), Abou Bekr-Belkaïd University, BP 119, Tlemcen, Algeria

[4]Physique departement, Faculty of Exact Sciences and Informatics, Hassiba Ben Bouali University, BP 151, Chlef 02000, Algeria

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** Corresponding author: a.bouhenna@univ-chlef.dz*

Key words : Porous material ; Equivalent fluid theory ; Transmitted waves ; Low frequency.

Abstract :

Over the past few decades, Heusler alloys have received particular interest, which is explained by different properties well suited to applications in spintronics devices, or spin electronics which is still relevant and in constant innovation. Its industrial potential is significant, such as hard disk reading heads, non-volatile magnetic random access memories (MRAM) and magnetic sensors. One of the properties that has contributed to the proliferation of work on these alloys is the semi-metallic character. Heusler alloys have many advantages that could adapt well to current technologies, such as strong magnetization, high Curie temperature and low magnetic damping. In addition to spintronic devices, Heusler alloys currently find several types of applications, notably in the thermoelectric field and superconductors(1).

In this work, we present the results obtained from studies carried out with the method of plane waves augmented and linearized with total potential (FP-LAPW) within the framework of the density functional theory (DFT) implemented in the WIEN2k code. The GGA approximation was used in calculating the structural properties of Heusler Co_2MnGe compounds, while the mBJ was used to calculate the electronic and magnetic properties. The results of the structural study of our materials have shown that they are more stable in the ferromagnetic (FM) phase than in the non-magnetic phase(2).

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CERAMIC SYNTHESIS AND CHARACTERIZATION OF NEW LANTHANUM-BASED ORTHOFERRITE CRYSTALS

A. Achour [1,], N. Zelikha[2] ,A. Malika[1], R. Rahima [1]*

[1] Laboratory of Molecular Chemistry and Environment, University of Biskra, B.P.145, 07000 Biskra, Algeria

[2] Laboratory of Applied Chemistry, University of Biskra, B.P.145, 07000 Biskra, AlgeriaAddress

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correspondence to E-mail: achouak.achour@univ-biskra .dz

Keywords : $LaFeO_3$, perovskite, ceramic, spectroscopic.

Abstract :

Lanthanum orthoferrite $LaFeO_3$, is an important oxide-type ABO_3 perovskite, where A = rare earth element and B = 3d transition metal.

The LaFeO3 unit cell consists of four formula units with Fe^{3+} ions surrounded by six O^{2-} ions in octahedral coordination resulting in an orthorhombic structure with a Pbnm space group [1]. Due to its attractive mixed ionic-electronic conductivity, $LaFeO_3$ has been proposed for many advanced technological applications, such as solid oxide fuel cells [2], oxygen sensors [3] and photocatalysts [4].

In this study, the doped $LaFeO_3$ powder was synthesized by conventional methods at high temperature (calcination and sintering).

The doped $LaFeO_3$ catalyst were prepared using commercial oxides, the $LaFeO_3$ calcined at 1000°C, and sintered at 1200°C. The structure and physical and chemical properties of our catalysts have been studied using techniques including powder X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectrometer (EDS), and FTIR spectroscopy.

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STRUCTURAL, MECHANICAL AND ELECTRONIC PROPERTIES OF A NEW α-PbO/α-SnO HETEROSTRUCTURE

A. Bakhtatou [1,*] *A. Hamidani*[1]

[1] *8 Mai 1945 Guelma University, BP 401 Guelma 24000, Algeria*

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** Corresponding author: bakhtatou.ali@univ-guelma.dz*

Keywords : Two-dimensional materials, α-PbO monolayer, α-SnO monolayer, Lateral heterostructures

Abstract :

Recently, monolayers of α-PbO and α-SnO have been experimentally synthesized with superior functionalities, making them industrially important material for many applications. However, we believe that the potential application of these monolayer materials could be further tailored when they are mixed together to form lateral heterostructures. In this study, we theoretically designed new lateral heterostructures (α-PbO)m/(α-SnO)m formed (for m=1 to 10) by periodically repeating narrow α-PbO and α-SnO strips joined along their adjacent one dimensional interface by first-principles DFT calculations. We have investigated the structural, mechanical and electronic of these heterostructures and shown that these structures could function as a forward p-n diode and can offer opto-electronic properties and quantum structures leading to device applications with interesting functionalities.

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ALUMINUM SUBSTITUTIONAL DOPING IN COPPER SULFIDE (Cu_2S) FOR INTERMEDIATE BAND SOLAR CELLS: A DENSITY FUNCTIONAL THEORY STUDY"

A. Madouri[1,], M. K. Benabadji[1,2], M. Benaissa[1,3], H. Si Abdelkader[1]*

[1]Laboratory of Materials Discovery, Unit of Research on Materials and Renewable Energies, LEPM-URMER, University Abou Bekr Belkaïd, B.P 119, Tlemcen, 13000, Algeria

[2]Laboratoire de Génie Electrique et Matériaux, Ecole Supérieure en Génie Electrique et Energétique d'Oran (Algeria)

[3]Université de Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000 Rennes, France

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* Corresponding author: Madouri.amine13@yahoo.fr

Keywords : Density Functional Theory, Doping, Intermediate Band gap, solar cells.

Abstract :

As the global energy crisis and environmental concerns persist, there is an escalating urgency to transition towards secure and renewable energy sources. Solar radiation stands as the foremost energy resource, necessitating the development of technologies that can efficiently harness solar energy, making it cost-competitive with fossil fuels. Metal sulfides, a fascinating class of semiconductors, known for their diverse technological applications in smart optical windows, solar cells, and gas sensors, have gained considerable attention. In the domain of cost-effective solar cell production, cuprous sulfide (Cu_2S), a prominent metal sulfide compound, emerges as a prime candidate due to its exceptional attributes: a high absorption coefficient, a direct band gap spanning 1.5 eV to 1.85 eV[1], abundant and non-toxic source materials, and easily scalable industrial fabrication processes [2].

To enhance the optical absorption capacity of a semiconductor, doping is utilized to introduce an intermediary electronic level, creating an intermediate bandgap material. In intermediate band photovoltaic technology, an energy level is inserted between the valence and conduction bands. Theoretically [3], this intermediate band enables an electron to transition from the valence band to the conduction band via the absorption of two photons with energies lower than the band gap, thereby increasing the photoelectric current and, subsequently, improving efficiency.

In this study, we employ density of states and optical properties simulations, utilizing density functional theory (DFT) [4], to investigate the feasibility of introducing an intermediate band level into cuprous sulfide (Cu2S) through aluminum (Al) doping. We also analyze the impact of this dopant on various physical properties of Cu2S, including structural arrangement, electronic structure, and optical characteristics. The insights gleaned from our findings can offer valuable guidance to researchers engaged in fabricating high-performance absorption layers for photovoltaic solar cells.

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FIRST-PRINCIPLES CALCULATIONS TO INVESTIGATE ELASTIC ANISOTROPY AND THERMODYNAMIC PROPERTIES OF HF-W LAVE PHASE

B.Dehina[1], I.K. Lefkaier[1]*

1Laboratoire de physique des materiaux, Ammar Thelidji University of Laghouat, Route de Ghardaïa,

B.P.73G,Laghouat, Algeria

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** Corresponding author:ba.dehina@lagh-univ.dz*

Keywords : intermetallic laves phase, DFT, Hf-W system.

Abstract:

Laves-phase intermetallic compounds have attracted great attention due to their excellent physicochemical properties, which make them potential candidates for many technological applications, such as superconductors and hydrogen storage materials. In this work, the structural, elastic, electronic, and associated dynamic and thermodynamic properties of the HfW_2 intermetallic Lave phase were investigated using first-principles calculations. The metallic conductivity is observed for the compound. The analysis of the bonding characteristicsof this compound reveals the presence of mixed covalent, ionic, and basic bonds. The estimated elastic constants were used to determine the Debye temperature of HfW2. The melting temperatures were computed and show good agreement with experimental values. The thermal conductivity of this compound was also predicted. Our findings provide valuable insights into the properties of Laves phase intermetallic compounds.

THE EFFECT OF DIFFERENT EXCHANGE CORRELATION ON THE ELECTRONIC STRUCTURE PROPERTIES OF LOW TEMPERATURE SILVER CHALCOGENIDE COMPOUND

H. Mancer[1,], A. Merrad[1], H. Rached[2,3]*

[1] Laboratory for Theoretical Physics and Material Physics, Faculty of Exact-Sciences and Informatics, Hassiba Benbouali University of Chlef, Chlef, Algeria

[2] Magnetic Materials Laboratory, Faculty of Exact Sciences, Djillali Liabes University of Sidi Bel Abbès, Sidi Bel-Abbès, Algeria

[3] Department of physics, Faculty of Exact-Sciences and Informatics, Hassiba Benbouali University of Chlef, Chlef, Algeria

** h.mancer@univ-chlef.dz*

Keywords : Electronic structures, Ag_2Se, DFT, GGA+U-mBJ.

Abstract:

The primary objective of this study is to examine how various exchange-correlation functional impact the electronic structures of low temperature silver chalcogenide compound β-Ag_2Se with space group P_{212121} (N° 19).[1] We have employed the (GGA, GGA+U, GGA+U-mBJ) fonctionals to calculate the exchange-correlation energy.[2] The band structure and density of states are determined through the utilization of the full potential linearized augmented plane wave (FP-LAPW) method, which is implemented in the WIEN2K code.[3] The calculation of the electronic structures indicate that, our compound exhibits a semiconductor behavior with an indirect band gap of 0.92 eV from GGA+U-mBJ calculation. This value agrees well with the experimental finding.

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ANALITIC STUDY OF THE EFFECT OF RADIATION BASED ON SILICON

K. Aouadj [1], D. Djamai [2] , M. Chahdi [1], S. Oussalah [3]*

[1]Batna 1 University, laboratoire d'études Physico-Chimiques des Matériaux LEPCM , Batna- Algeria

[2]Khenchela University, laboratoire d'Ingénierie et Sciences des matériaux Avancés ISMA, Elhamma- Algeria

[3] Centre de Développement des Technologies Avancées CDTA, Division Microélectronique et Nanotechnologies, Algiers - Algeria

** Corresponding author: Khaoula.aouadj@univ-batna.dz*

Keywords : HL-LHC, ITk, Silicon, Pixel.

Abstract :

The Large Hadron Collider (LHC), located at CERN, Geneva, produces accelerated proton collisions with an energy of 3.5 TeV. In 2012, the LHC project achieved a remarkable success with the discovery of the Higgs boson. However, the project is not yet finished, and aims to go even further in the search for new physics and high-precision measurements. The plan is to increase the beam's instantaneous luminosity to 7.5×1034 cm-2 s-1 to move into the high- luminosity phase (HL-LHC). This means that the internal trajectograph will not be able to cope with such an increase in stacking and radiation rate. In order to maintain the same performance of the ATLAS inner detector, the current tracker will be replaced by a new one entirely made of silicon, called Inner Tracker (ITK), based on the insertion of silicon pixel sensor layers. Silicon detectors are the only type of detectors capable of being efficient and surviving the harsh conditions expected for HL-LHC. In this work, we present a comparative study using TCAD Silvaco tools of n-on-p planar pixel sensors, before and after irradiation.

FIRST PRINCIPLE STUDY OF THE STRUCTURAL, ELECTRONIC AND THERMODYNAMIC PROPERTIES OF CrCoLaZ alloys (Z=Ga; Si)

H. Kamel[1], G. Youcef [1], M. Ahmed[1]

[1]Thin-film physics and advanced technologies laboratory, University of Relizane, Algeria

** Hocine Kamel: hocine_kamel@yahoo.com*

Keywords : Heusler, electronic properties, thermodynamic properties, half-metal

Abstract :

An ab-initio calculation was performed using the linearized augmented plane wave method (FP-LAPW), within the framework of density functional theory (DFT), with the generalized gradient approximation GGA to calculate the structural, electronic and magnetic properties of quaternary Heusler CrCoLaZ alloys (Z=Ga, Si) which are of technological interest in the field of spintronics research. Calculations show that CrCoLaZ (Z=Ga, Si) compounds having characteristics of ferromagnetic half-metal with a gap of 0.6 eV. Using the quasi-harmonic Debye model, the variations of lattice parameter, thermal expansion coefficient, heat capacities and Debye temperature with pressures covering the 0–20 GPa interval and temperatures ranging from 0 to 1200 K were also investigated and in-depth discussed. The results of our simulation have been interpreted and compared to the theoretical results available.

STRUCTURAL, ELECTRONIC, AND OPTICAL PROPERTIES OF DOUBLE HALF-HEUSLER ALLOY

H. Mekki[1,2], H. Baaziz[1,2], Z. Charifi[1,2], T. Ghellab*

[1] Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria

[2] Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria

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** Corresponding author : houria.mekki@univ-msila.dz*

Keywords : Double half Heusler, DFT, Optoelectronic.

Abstract :

The orthorhombic structure of the double-half Heusler compound $ScNbNi_2Sn_2$ was examined by first-principles calculations employing the full-potential linearized augmented plane wave method (FP-LAPW) [1]. These calculations were based on density functional theory (DFT) [2-3]. The utilization of the generalized gradient approximation (GGA) [4] is employed for the treatment of the exchange-correlation potential, while the EV-GGA [5] is utilized to enhance the band gap in order to evaluate the structural, electrical, and optical features.

This study presents an analysis of the computations for our compound indicating that the GGA approximation with the nonmagnetic state yields the lowest energy. Therefore, it can be inferred that the GGA approximation is the most suitable for accurately describing the structural features. The band structures obtained by computation exhibit semiconductor behavior, characterized by an indirect bandgap of 0.47 eV, as determined through the use of the EV-GGA approximation. In addition, an examination was conducted on the optical characteristics, including the dielectric function, optical conductivity, and refractive index.

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STRUCTURE, ELASTIC, MECHANICAL, ELECTRONIC AND MAGNETIC PROPERTIES IN PALLADIUM-BASED FULL-HEUSLER ALLOYS Pd_2MnZ (Z = Al, Si): *AB INITIO* CALCULATIONS

H. Bouchenafa [1,], B. Benichou [2,3], B. Bouabdallah [3], Z. Nabi [3]*

[1] Laboratory for Theoretical Physics and Material Physics, Faculty of Exact Sciences and Informatics, Hassiba Benbouali University of Chlef, 02000 Chlef, Algeria

[2] Department of Electronics, Faculty of Technology, Hassiba Benbouali University of Chlef, Chlef 02000, Algeria

[3] Computational Materials Physics Laboratory (CMPL), Faculty of Exact Sciences, Djillali Liabès University of Sidi Bel Abbès, Sidi Bel Abbès 22000, Algeria

**Corresponding author: bouchenafa_halima@yahoo.fr*

Keywords : Heusler alloys, Ferromagnetic, metal, ab initio calculations.

Abstract :

We used the full-potential linearized augmented-plane wave (FP-LAPW) approach within the density functional theory (DFT) as included in the WIEN2k program to explore the electronic structure, magnetic, and mechanical features of the ternary full-Heusler compounds Pd_2MnZ (Z = Al, Si). Forthe exchange-correlation functional, the generalized gradient approximation (GGA) is employed. The equilibrium lattice constants and spin magnetic moments are in close agreement with the experimental measurements and theoretical calculations. The band structures and density of states (DOS) of the studied alloys show a ferromagnetic metallic behavior. Furthermore, based on mechanical stability conditions, our predicted elastic constants show that the Pd_2MnSi Heusler alloy is mechanically stable in an $L2_1$-type structure, anisotropic, and ductile, whereas Pd_2MnAl is not. Finally, we hope that our findings will serve as a foundation for future research.

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AB-INITIO STUDY OF THE PROPERTIES OF $Tl_2PdFe(Ru)Sb_2$DOUBLE HALF-HEUSLER SEMICONDUCTING ALLOYS FOROPTOELECTRONIC APPLICATIONS

M. Diaf[1], H. Righi[1], H. Rached[2,3], D. Rached[2]*

[1] Laboratory of Physical and Chemical Studies of Materials (LEPCM). Faculty of Matter Science , Department of Physics, University of Batna 1, Batna, Algeria

[2] Materials Laboratory (LMM), Faculty of Exact Sciences, Djillali Liabes University of Sidi Bel- Abbes, Sidi Bel- Abbes, Algeriaor

[3]Department of Physics, Faculty of Exact Sciences and Informatics, Hassiba Benbouali University of Chlef, Chlef,Algeria

** Corresponding author e-mail: mohamed.diaf@univ-batna.dz*

Keywords : Double half-Heusler alloys, semiconductors, ab-initio, elasticity, electronic and optical properties

Abstract :

Using ab-initio calculations, we have studied the structural, mechanical, electronic and thermoelectric properties of the new double half-Heusler alloys[1,2], $Ti_2PdFeSb_2$ and $Ti_2PdRuSb_2$.

Our calculations predict stable non-magnetic semiconducting phases with indirect band gaps of 0.9eV for $Ti_2PdFeSb_2$ and 0.7eV for $Ti_2PdRuSb_2$. The calculated formation energies and elastic constants suggest that both alloys are thermodynamically as well as mechanically stable. By analyzing the optical properties (dielectric function, optical conductivity, refractive index, absorption index and reflectance), our calculations suggest that both materials have high absorption coefficient and optical conductivity in the UV as well as visible region. The collected results suggest that both compounds would be potential candidates for for the manufacture of

photovoltaic devices.

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THERMOELECTRIC PROPERTIES OF ZINTAL COMPOUNDS BY AB INITIO CALCULATIONS

I. Mili[1,2] H. Latelli[1,2]T. Ghellab, Z. Charifi[1,2], H. Baaziz[1,2]*
[1] Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria

[2] Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria
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** Corresponding author: charifizoulikha@gmail.com*

Keywords : Zintl compounds; electronic structure; thermoelectric materials; figure of merit; Seebeck coefficient..

Abstract :

The investigation focuses on the examination of the physical properties of $Ca_{1-x}Yb_xZn_2Sb_2$ (x = 0, 0.25, 0.5, 0.75, 1) Zintl compounds taking into consideration their electronic structure. The transport properties can be significantly changed by varying the composition x. the transport characteristics can undergo substantial modifications. The materials being investigated exhibit greater metallic properties as the value of x increases, while demonstrating semiconductor behavior when x lowers. It has been discovered. The compound $CaZn_2Sb_2$ has a significantly greater magnitude (S = 241 µV/K at T = 700 K) and the Seebeck coefficient decreases as x increases. The calculated figure of merit factor of YbZn2Sb2 is found to below, this is explained by the fact that its structure is very compact and its bandgap is small which lead to high electrical and thermal conductivity due to high carrier concentration (n = 1.25 $x10^{20}$ cm^{-3} at T = 300 K). On other hand a narrow-gap (0.46 eV for $CaZn_2Sb_2$), provides a balance between a high Seebeck coefficient and low electronic thermal conductivity, with a slight increase in the carrier concentration when the temperature increases (3.87x 10^{19} cm^{-3} at 600 K). As a consequence, $CaZn_2Sb_2$ compound is predicted to have good performance for thermoelectric applications. The electrical (σ) and the thermal (K) conductivity for $CaZn_2Sb_2$ compound in both directions (along x and z-axes) are calculated. It is obtained that (σ_{xx}) is 120% of (σ_{zz}) at high-temperature, whereas S_{zz} Seebeck coefficient was higher than S_{xx} especially at T = 300 K (S_{zz} = 246 µV/K, S_{xx} = 213 µV/K). The large value of S_{zz} showed that the transport is dominated by zz-axis.

UTILIZING GENETIC ALGORITHMS TO DETERMINE OPTIMAL HYDROGEN POSITIONS IN CUBIC CU_2S FORENHANCED SOLAR CELL PERFORMANCE

M. Benaissa[1,2,], T. Ouahrani[3], H. Si Abdelkader[2], D. Sébilleau[1]*

[1]Université de Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000 Rennes, France

[2]Laboratory of Materials Discovery, Unit of Research on Materials and Renewable Energies, LEPM-URMER,University Abou Bekr Belkaïd, B.P 119, Tlemcen, 13000, Algeria

[3]École supérieure en sciences appliquées, ESSA-Tlemcen, BB 165 RP Bel Horizon, Tlemcen 13000, Algeria.

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** Corresponding author: med.benaissa.dz@gmail.com*

Keywords : Genetic algorithms, Cu_2S, solar cell, hydrogen doping, Density Functional Theory

Abstract :

In the quest of cutting-edge and economically feasible materials to enhance solar cell technology, Copper sulfide (Cu_2S) emerges as a prominent frontrunner, driven by its highly advantageous optical and electronic characteristics coupled with its abundance [1–3]. Given the ever-increasing global appetite for sustainable energy resources, the imperative for such materials has attained unparalleled significance. Cu_2S unequivocally manifests an exceptional capacity for proficiently harnessing solar radiation and effecting its conversion into electrical energy, thus establishing itself as a cornerstone in expediting the transition toward environmentally conscientious and sustainable energy solutions.

During the intricate fabrication process of Cu2S, hydrogen is naturally incorporated into its crystal lattice. This seemingly spontaneous integration of hydrogen introduces an element of complexity and intrigue, as it significantly alters the material's characteristics [4]. The interactions between hydrogen atoms and the Cu_2S lattice hold the key to unlocking enhanced solar cell performance. However, understanding and manipulating these interactions remain elusive and challenging within the realm of experimental settings.

In response to this challenge, our article introduces a novel and sophisticated approach. We combine the power of genetic algorithms [5] with the precision of Density Functional Theory (DFT) calculations [6] to identify the optimal positions for hydrogen incorporation within the cubicCu2S structure. Our research will guide experimentalists seeking to delve into the profound effects of hydrogen on Cu2S properties, particularly in the context of solar cell applications.

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NUMERICAL SIMULATION AND EXPERIMENTAL VALIDATION OF DUCTILEDAMAGE MODEL AND APPLICATION TO DEEP DRAWING PROCESS

S. Laboubi[1,] O. Boussaid[2]*

[1] *Laboratory of Metal Materials Forming, Badji Mokhtar University, BP.12,23000 Annaba, Algeria*

[2] *Laboratory of Research on Industrial Risks, Control and Safety, Badji Mokhtar University, BP.12,23000 Annaba,Algeria*

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* *Corresponding author: salah.laboubi07@gmail.com*

Keywords: Ductile damage, Numerical simulation, Ductile fracture, Deep drawing process.

Abstract :

The present work discusses the ability of Lemaitre ductile damage model to predict the thinning and fracture of DC04 sheet metal during the deep drawing process. In this model, the elastoplastic constitutiveequations considering isotropic and anisotropic plasticity coupled with isotropic damage have beendeveloped and implemented in the Abaqus Explicit code using the VUMAT subroutine, knowing that the elastoplastic and damage parameters of the used material have been identified by experimental tests. In order to verify the accuracy of this model, several numerical simulation scenarios have been performed, and their results are compared with the experimental results. These comparisons show a good correlation between the experimental and simulation results and good agreement with the empirical observations. Thus, the used model is valid to predict the elastoplastic-damage behaviour of the sheet metals during the forming process and can well localise the thinning and fracture.

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INVESTIGATING THE PHYSICAL PROPERTIES OF $RbXF_3$ (X =Rh, Os, Ir, V) COMPOUNDS

Ş. Uğur[1,], Y. Uysal[1], M. Güler[2]*

[1] *Gazi University, Department of Physics, 06500 Ankara, TURKEY*

[2] *Ankara Hacı Bayram Veli University, Department of Physics, 06900 Ankara, TURKEY*

* *Ş. Uğur: suleugur@gazi.edu.tr*

Keywords : Band gap, rubidium-based fluorides, elastic properties, ferromagneticsemiconductor.

Abstract :

The structural, elastic and phonon properties of $RbXF_3$ (X = Rh, Os, Ir, V) compounds were explored by performing first-principles calculations within the generalized gradient approximation (GGA). Spin-polarized band structure calculations for the $RbXF_3$ (X = Rh, Os, Ir, V) compounds have been investigated. The results for the electronic band structure and density of states agree with existing literature data[1,2]. Likewise, the optimized lattice parameters and elastic constants display reasonableresults compared to previous works[1,2]. Optical properties were also calculated along [100] polarization under energies up to 50 eV. From the results of the optical response, it is found that these compounds show high optical absorption in the broad range of 5 eV to 30 eV.

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INVESTIGATION OF THE STRUCTURAL, ELECTRONIC, ELASTIC AND OPTICAL PROPERTIES OF $InGeCl_3$, $InSnCl_3$ AND $InPbCl_3$ COMPOUNDS

Ş. Uğur[1,], B. Dağdeviren[1], E. Güler[2]*

[1] *Gazi University, Department of Physics, 06500 Ankara, TURKEY*

[2] *Ankara Hacı Bayram Veli University, Department of Physics, 06900 Ankara, TURKEY*

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* *Ş. Uğur: suleugur@gazi.edu.tr*

Keywords : Perovskite compounds, elastic constants, optical properties, density of states.

Abstract:

This work reports the structural, elastic, electronic and optical properties of $InGeCl_3$, $InSnCl_3$ and $InPbCl_3$perovskite compounds determined by the first-principles method. The generalized gradient approximation(GGA) of Perdew-Burke-Ernzehrof (PBE) was used for all calculations. The elastic constants were predicted using the static finite strain method. Using the obtained elastic constants C_{ij}, the bulk modulus (*B*), Young's modulus (*E*), shear modulus (*G*), Poisson's ratio (*v*) and Pugh's ratio (*B/G*) of $InGeCl_3$, $InSnCl_3$ and $InPbCl_3$ were calculated. Electronic band structures and density of states calculations show that all these compounds possess a semiconducting nature. The estimated lattice parameters and band gap values match the previous studies[1,2]. Finally, the optical properties of the titled compounds were also analyzed in detail.

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STRUCTURAL, ELECTRONIC, MAGNETIC AND THERMODYNAMIC PROPERTIES OF VSIRH2: A DFT STUDY

S. Makhlouf[*], *M. Labidi*, *A. Amara*

Department of Physics, LEREC Laboratory, Badji Mokhtar University, Annaba, Algeria

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** Corresponding author: sabir.makhlouf@gmail.com*

Keywords : DFT, Wien2k, Thermodynamic, Debye temperature, VSiRh2, Heusler.

Abstract :

This study investigates the Structural, Electronic, Magnetic and Thermodynamic properties of full-Heusler alloy VSiRh3, Our research employs DFT method integrated into the Wien2k code. The results obtained show the ferromagnetic stability for VsiRh3 and constant of lattice is found to be 6.04 Å, usingPBE-GGA method based on DFT for the optimization. SCF calculation and modified Becke and Johnson (mBJ), represented by BS and DOS, revealed the metallicity of VSiRh3. We used the Gibbs2 code to delve into the thermodynamic properties of VSiRh3. The valence wave functions were expanded up to
L_{max}=14 partial waves. We set $R_{mt}K_{max}$ to 8, G_{max} to 14 $a.u^{-1}$, and utilized a dense $(14 \times 14 \times 14)$ k-point mesh. The total energy convergence was set to a high precision of 10^{-6} Ry. We obtined the totalspin magnetic which is 3.28 mB. Moreover, debye temperature, constant-volume heat capacity and entropy are calculated from 0 to 500 K.

STRUCTURAL, ELASTIC AND ELECTRONIC PROPERTIESOF DOUBLE PEROVSKITE Ba_2NaIO_6AN AB INITIO CALCULATIONS

S..MENDER[1], S.LABIDI[1]

[1] Laboratory of Nanomaterials, Corrosions and surface traitements , Department ofPhysics, Faculty of Sciences, University of Badji Mokhtar, BP 12, 23000 Annaba, Algeria.

Mendersara1@gmail.com

Keywords :

Ba_2NaIO_6;DFT; FP-LAPW; mBJ(GGA); electronic , propertie.

Abstract :

Structural, elastic and electronic properties for Ba_2NaIO_6 compounds in cubic structure were studied usingdensity functional theory and Wien2k code. For the generalized gradient approximation (GGA) of exchange correlational functional as parameterized by Perdew Burke and Erenzerhof (PBE) beside employing modified Becke- Johnson (mBJ) approximations were used. Various quantities, such as equilibrium lattice constants, bulk modulus and band structures are presented, and this values agree well with the available literature results.The Ba_2NaIO_6 possesses a direct bandgap, according to the electrical structural studies.

AB-INITIO" STUDY OF THE STRCUTCURAL ELECTRONIC AND THERMODYNAMIC PROPERTIES OF PREVSKITE OXIDE $MoScO_3$

B.Sehoul[1,], S.Bouguerba[1], M.Sehoul[1]*

[1]Laboratory of electronic systems, telecommunications and renewable energy, Nour-El Bachir University Center,BP900, El-Bayadh, 32000, Algeria

** Corresponding author: sehoulbaghdad2019@gmail.com*

Keywords: Ab-initio Calculations, density functional theory, GGA, $MoScO_3$.

Abstract:

The subject of this work concerns the study of the structural, electronic and thermodynamic properties of the perovskite oxide $MoScO_3$.using the full potential linearized augmented plane wave method (FP-LAPW) in the frame of density functional theory (DFT) which is implemented in the wien2k code[1]. The exchange-correlation effects are treated with the GGA[2] with the mbj approximation. The results obtained showed that the studied compound $MoScO_3$ is stable in the ferromagnetic (spin polarized).for electronic properties; our results indicated that the studied compound has a semi-metallic (semiconducting and metallic in the minority and majority spins respectively. We completed this work by studying thethermodynamic properties through variation in heat capacity, the compressibility coefficient at different pressure using the Debye quasi-harmonic model[3]

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STUDY OF PHYSICAL PROPERTIES BASED ON SP-DFT THEORY FOR CO-DOPED MGO WITH Eu-Tm.

T.*Wissem,*[1] C. Sabahr*[1]

[1] *Laboratory of materials Physics , University May 8 1945, Guelma, Algeria*

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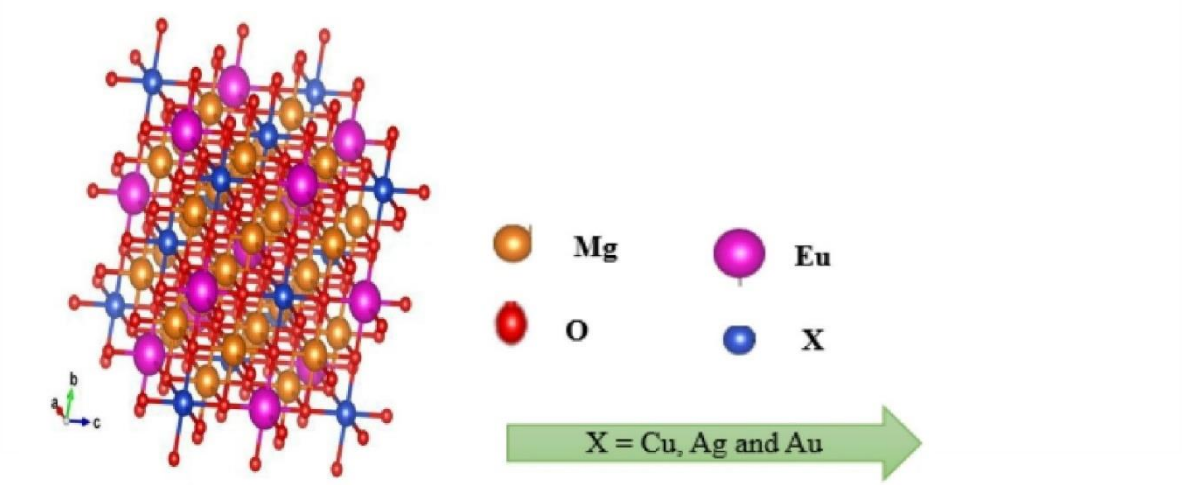
** Corresponding author: tayeb.halais782@gmail.com.*

Keywords : Ab initio calculations, MgO, Rare Earth, Physical Properties

Abstract:

This work analyzes how adding europium and transition metals (Cu, Ag, and Au) at a 12.5%

concentration to magnesium oxide (MgO) affects it's structural, magnetic, and optoelectronic properties. The full potential linearized augmented plane wave (FP-LAPW) method, based on spin-polarized density functional theory (SP-DFT), is used to derive results. The produced dilute magnetic oxides (DMO) are stable in the ferromagnetic phase when Eu and TM (Cu, Ag, and Au) impurities are co-doped into the non-magnetic semiconductor MgO. This theoretical work paves the path for the creation of a high magnetic moment DMO suited for spintronic and UV devices using TM and rare earth as dopants.



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AB INITIO STUDY OF STRUCTURAL, ELECTRONIC, MAGNETIC AND THERMODYNAMIC PROPERTIES OF FeNi ALLOYS.

*Z. Zine[1],**

[1] Department of physics, Faculty of Exact Sciences, University of El-Oued, 39000 El-Oued, Algeria

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** Corresponding author:Zinezine177@gmail.com*

Keywords : FPLAPW, WIEN2k , density functional theory (DFT) ,DOS.

Abstract :

Electric power generators, motors, and transformers are just a few examples where magnetic materials find an application in modern technology.
The ordered FeNi phase (tetrataenite) is recently considered as a promising candidate for the rare-earth free permanent magnets applications, To investigate the electronic and magneticproperties of FeNi structures, a computational approach based on the full potential linearized augmented plane wave (FPLAPW) method was employed which is based on density functional theory (DFT) These calculations were performed using the WIEN2k software package .
Structural properties obtained as the lattice parameter are in good agreement with the experimental results available and Other theoretical studies. From the electronic band structure along with total and projected DOS, we conclude that FeNi shows metallic nature with a significant contribution of 3d-Fe and 3d-Ni states to the total electronic density of states. In addition, studies on the Thermodynamic properties of FeNi alloys indicate that The volumetric thermal expansion coefficient is an important parameter to measure the thermal stability of the alloy.
FeNi alloy always has the smallest volumetric thermal expansion coefficient at the same temperature and pressure, indicating that this alloy has the best thermal stability. shows the Debye temperature versus temperature at different pressures of FeNi alloys.where the FeNi alloy has a high Debye temperature at high temperature, indicating that this alloy has the highest melting point at normal pressure.

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EXPERIMENTAL CHARACTERIZATION OF STEEL CORRODED IN HCL ASAGGRESSIVE SOLUTION.

A. Hamada[1], L. Saouli[2], K. Oulmi [2]

[1]Department of Process Engineering, Faculty of technology, University of Batna 2, Algeria

[2]Laboratory of Chemistry and Environmental Chemistry, Department of Chemistry, Faculty of Science, Universityof Batna, Algeria

[1] a.hamada@univ-batna2.dz,

Keywords: Aggressive solution, corrosion, materiel, steel.

Abstract:

Excellent mechanical properties make carbon steel (A60) an essential material which is used in various fields, including maritime and petroleum sectors A60 steels are easily corroded in acidic environments, mainly in hydrochloric acid used for industrial pickling, acid scaling, cleaning and acidification of oil wells. The annual cost of losses could be estimated at several billion dollars. Although many solutions such as coatings and deposits were proposed to prevent metals from corroding, the use of corrosion inhibitors remains among the best and most effective means Corrosion inhibitors are distinguished by their high adhesion capacity on metal surfaces. The rate of corrosion is immediately reduced when the inhibitor is added since it quickly prevents corrosion .

The choice of inhibitors to be studied must be made according to three essential criteria, namely, its richness in antioxidants, its abundance in nature and its cost. The inhibitors used in this work are extracts of Ginger and Turmeric plants.

Characterization methods such as gravimetric technique (mass loss) and electrochemical technique (potentiodynamic polarization) were used to measure corrosion rates.

For the Gravimetric Technique, it determines the mass loss. Measurements of mass loss (m) in a surface sample (S) during a time of immersion (t) in a corrosive solution at constant temperature.

The aggressive medium is hydrochloric acid 1,5 M solution to which various concentrations of ginger and turmeric powder are added as inhibitors.

The current-voltage curves confirm the indications given by the evolution of the corrosion potential as a function of time and those of the lost mass; estimate the corrosion rate and the influence of the inhibitor on each of the anodic and cathodic elementary reactions of the working electrode. This method determines accurately the electrochemical parameters of a metal in contact with an electrolyte, namely: current density (i_{corr}), corrosion potential (E_{corr}), Tafel slopes (β_c andβ_a) and polarization resistance (R_P).

The obtained results have direct implications on the development of corrosion-resistant materials and on the design of protection solutions. This research may allow a better understanding of the complex interactions between materials and their corrosive environment, and may help to innovate in corrosion prevention and improve material durability.

ANCIENT ALLOYS BASED ON GOLD, GENERALITIES AND CASE STUDIES.

*Z. BACHI ,*BENBERKANE. Saadia,*

University of Batna1, Algeria
** zineddine.bachi@univ-batna.dz*

Key words: Ancient alloys, gold, electrum coin, Metallography, numismatics

Abstract: Contents in major elements (gold, silver, copper) could be checked, even in ancient times (by touchstones for example), many other elements are present in ancient gold coins at low contents. They come from: The gold ore (type of ore, provenance) / Gold recycling / Alloying of gold with silver and copper (which contain their own impurities)

The contents in major, minor and trace element may inform us on the coins production and on the questions of gold provenance "stocks" of gold used. So we wonder what the method is used to determine the quality of the minted alloy: proportion of precious metals such as gold? And how can we analyze gold coins and what are they used for?

- How purified is gold? What is the standard of purity?
- How was gold debased? Could debasement remain more or less hidden (colour, weight, volume)?
- Were different series of gold coins struck from the same gold stock? Was a series of coins melted down to strike a new series of coins?

Detection of gold alloy through Elemental analysis, Isotopic analysis and Metallography; There are historical stages in which gold was not purified to a large extent, being limited to recycling of used gold, especially with the decline of sources of raw gold in nature.

Due to the expansion of the old empire, limited sources of raw gold, and the lack of sufficient mints to mint gold coins, other elements were added to the raw gold alloy in order to fill the shortage, particularly with regard to the payment of salaries, nobles and military leaders.

In later periods the emphasis was on gold and silver alloys in varying proportions of up to 70%.

From the archaeo-numismatics study, we will be able to know about coins analysis:

• Elemental analysis	• Isotopic analysis	• Metallography
Qualitative / Semi-quantitative / Quantitative/ Destructive / Non-destructive/	Mostly the determination of the ratios between the 4 stable isotopes of lead. For provenance studies: comparison of samples of the same type or with geological data (ores).	Destructive: study of polished cross-sections, Information about the micro-structure of the alloy.

In all cases, Analysis are not carried out for themselves, A clear historical/archaeological question needs to be defined prior to the analysis for determining which method would be adapted, its cost and availability, if it is invasive/destructive or not, The interpretation should rely on the analytical results. Through our research, we found that; Determination of the alloy quality of the minted alloy (proportion of the precious metals, at least gold)

Byzantine gold coins 491 to 1180 lead for tracing the additions of silver metal to gold[1] :

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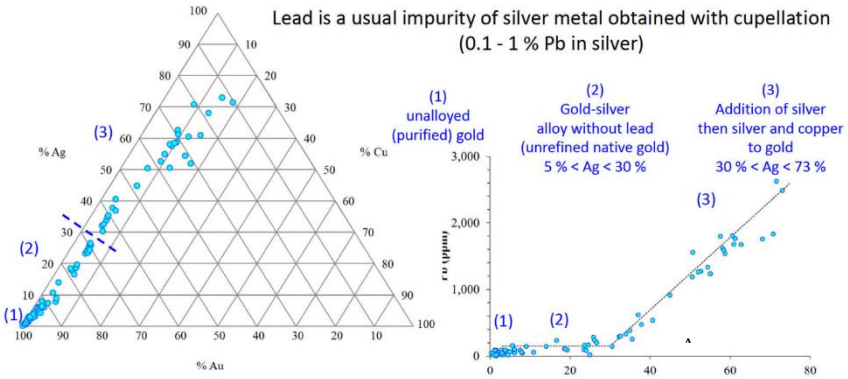

INVITED SPEAKERS

Pr. Zoulikha Charifi

University of M'sila, Algeria

Prof.Dr. Hafid Aourag

Prof.Dr. Vallery Vassiliev

Lomonosov Moscow State university (Russia)

Prof.Dr. Gokay Uğur

Gazi University (Turkey)

Prof.Dr. Emre Güler

U. A. Haci Bayram Veli (Turkey)