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PREFACE

The world of nanomaterial science is moving forward really fast, covering such a wide range of areas that it's a real challenge for anyone to keep up, unless you're completely into the subject. To deal with this, universities and industries have to work hard to inspire the next generation of scientists and engineers, giving them the essential skills to handle the challenges of this new era.

The main goal of the NSN'24 conference is to thoroughly explore the big picture of nanomaterials and all the different things they can do. Most importantly, we want to make it easy for researchers who are really into this stuff to share their experiences and knowledge on a national level. The scientific program of the seminar is carefully put together, with interesting talks, discussions, oral presentations, and poster sessions. Nanomaterials, because they can be used in so many different ways, offer a bunch of opportunities in areas like microelectronics, pharmaceuticals, and clean energy.

This scientific event is dedicated to the innovative field of nanomaterials, with particular emphasis on their various applications. This event will serve as a catalyst for advancing the field of nanomaterials, thereby making notable contributions to interdisciplinary research in this area. As we immerse ourselves in the exciting and innovative world of nanomaterials, we anticipate this conference will play a pivotal role in shaping the future of this dynamic field in our country.

CONFERENCE TOPICS

1. Nanomaterials Elaboration & Characterization
2. Nanomaterials for Environmental and Sustainable Energy
3. Nano-Technologies & Nano-Electronics
4. Nano-Medicine & Nanobiology
1. Simulation and Modeling of Nanomaterials

PLENARY LECTURES

Pr CHAKNANE ALI

Department of Electrical Engineering, Faculty of Sciences and Engineering Sciences, Amar Telidji University of Laghouat, BP 37G, route de Ghardaïa, LAGHOUAT (03000) ALGERIA

Magnesium hydride nanoparticles for hydrogen storage

Pr HATEM DJEDJIGA

Department of Electronics. Discipline Department of Electronics. Disciplines. Thin Films • Solar Cells • Materials, Mouloud Mammeri University of Tizi Ouzou, ALGERIA

Clean and sustainable nanomaterials and processes for energy and microelectronics

Abstract

The emergence of modern microelectronic devices has accelerated research into high-performance rechargeable microbatteries. Lithium-based systems respond better to the voltage and energy density requirements of microbatteries. At present, it is necessary to move on from the conventional configuration (2D) to the new three-dimensional nanostructured configuration (3D) and adopt the 'lithium-ion' or 'rocking-chair' concept.

Among the vast range of anode materials that can react reversibly with lithium, nanotubes are the most promising.

The initial works focused mainly on the development of titanium dioxide nanotubes (TiO2 NTs) using the electrochemical titanium anodisation process, while optimising the synthesis parameters such as anodisation voltage, dwell time, H2O content and electrolyte type. Next, the modification of the physical properties of nanotubular titanium oxide and thus the improvement of electrochemical performance and the obtaining of self-organised TiO 2 NTs while incorporating dopants for use in lithium micro-batteries application to improve energy storage efficiency.

Pr NADJIB BAADJI

Department of Physics, University of M'sila, Algeria

Nanomaterials and nanotechnology from theoretical perspectives

Abstract

Nanotechnology is one of the most significant research area and it is the fundamental technology of the industrial revolution of 21st century. It has found huge applications in several sectors such, in medicine (as medical equipment like imaging probes, drug delivery systems, and diagnostic biosensors), in nano-electronics (devices for information storage and processing) and many other area. The nanoscale systems, where at least one of the system dimension is nanometric, must be addressed with quantum concepts, and it presents physical properties that differ significantly from their bulk counterparts. In this talk, we will address the use of the density functional theory for describing the nano-materials, its success and its limitations. We will describe how to use the non-equilibrium Green's function (NEGF) formalism to calculate the transport properties of magnetic and molecular junctions. Finally, we will highlight the need to go beyond the mean field theory to investigate low temperature phenomena observed in quantum dots, like the Kondo and Fano effects.

Pr. YAHIAOUI KARIMA

Laboratory of food Technology, Boumerdes, Algeria

Nanoparticles in the food industry: benefits and challenges

Abstract

The use of nanoparticles in the agri-food sector has increased significantly in recent years. These nano-sized particles offer a number of advantages for the industry. Technologically, they can be used to improve various food properties, such as texture, colour and

preservation. Nutritionally, nanoparticles can also be used to encapsulate and protect sensitive nutrients, thereby improving the bioavailability of micronutrients. However, the increasing use of these nano-additives in the food industry is raising concerns about their potential impact on food quality and consumer health. Their small size enables them to cross biological barriers more easily, raising questions about their potentially harmful effects. Some studies have highlighted the risk of organ toxicity and negative impacts on the immune system. As a result, the use of these nano-additives in foodstuffs needs to be strictly regulated and supervised to guarantee consumer safety. In-depth research is also essential to better understand and quantify the long-term impact of these nanoparticles on human health.

ABAIDIA SADDIK EL HAK

Laboratoire Revêtements, Matériaux et Environnement, Université de Boumerdès, Faculté des Sciences

Development of nanomaterials in the field of energy efficiency,

ecology and human comfort: the case of modern housing

Following the first oil crisis in 1973, there was a demand to reduce the energy consumption of buildings. To reduce heat loss, various developments led to a spectacular increase in the thermal insulation of external walls, whether brick or concrete block walls, as well as glazed surfaces.

Windows and glazing have followed a similar trend, with significant improvements in heat loss coefficients. For example, the replacement of single glazing with double glazing in the 1970s had already halved heat loss. Next came the first glass with thermal coatings (ultra-thin surface treatment), followed by ever thinner layers of insulation, combined with thermally insulating gases placed between the 2 panes. These modern double glazed units offer 5 times the thermal performance of the old single glazed units, which are now totally obsolete...

The energy efficiency of glazing is based on the concept of "energy balance", which takes into account the difference between heat loss (from the inside to the outside) and energy gain (from the outside to the inside) due to solar radiation.

Pr. YAHIAOUI KARIMA

Laboratory of food Technology, Boumerdes, Algeria

Pesticide VS nanopesticide: a real opportunity for agriculture

The debate between traditional pesticides and nanopesticides represents a real opportunity for agriculture. While conventional pesticides have long been used to protect crops, there is growing concern about their impact on the environment and human health. Nanopesticides, on the other hand, are nanotechnology-based pesticides that offer improved properties such as controlled-release systems and enhanced efficacy.

Nanopesticides have several potential advantages. They can be designed to be more targeted and pest-specific, reducing the amount of product needed and minimising losses through leaching and drift. In addition, they can be modulated to release active ingredients in a controlled manner as required, optimising their efficacy and reducing short-term environmental impacts.

However, it is important to bear in mind the potential harmful effects of nanopesticides. The materials used in their manufacture can have toxic effects on plants, humans and other vertebrates due to their biomimetic properties with the cell wall. It is therefore essential to conduct in-depth studies into their safety and environmental impact before using them on a large scale.

ORAL

PRESENTATIONS

Microscopic Insights into Failure Mechanisms and mechanical properties of a PLA Biocomposite with Natural Fiber Reinforcement

Khalil Benabderaza, Moussa Guebailia
University of Ouargla
Corresponding author: khalilstts@gmail.com

Abstract:
This study investigates the fracture morphology of a biocomposite composed of a PLA matrix and Lygeum spartum L. fiber reinforcements. Scanning electron microscopy (SEM) was employed to analyze the cross-section of the fractured surface. SEM images revealed the fiber distribution within the matrix and variations in fiber structure, including the presence of both bulk fiber formations and individual elementary fibers. Crucially, the images also displayed micro- and nanoscale marks on the fibers. These marks are indicative of failure mechanisms under stress, such as matrix cracking, fiber pullout, and fiber debonding. This detailed morphological analysis provides valuable insights into the biocomposite's behavior and deformation mechanisms under applied stress.

Keywords: Biocomposite, PLA, natural fiber, fracture morphology, scanning electron microscopy (SEM), failure mechanisms.

Study of the inhibitory effect of nickel oxide nanoparticles on the corrosion of carbon steel X70

Saliha Bougherara, D. Cherik, F. Lecheb, M. Belkhir , S. Smaili, F. Aissat, K. Deleci, L.Neggache , A. Dremchi
Faculty of Technology, Boumerdes University
Corresponding author: boughrarasaliha@yahoo.fr

Abstract:
During this study, we synthesized Nickel oxide nanoparticles (NiO NPS) to use them as a corrosion inhibitor for X70 carbon steels. During this work, we analyzed the phase structure, crystallinity, surface morphology and other characteristics of NiO NPs produced using different techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM). , X-ray fluorescence (FX) analysis and X-ray diffraction (EDX). Subsequently, we studied the electrochemical corrosion behavior of NiO NPs in the presence of an aqueous electrolyte containing NaCl at a concentration of 0.6 Mol/l.

Keywords: Nickel oxide nanoparticles (NiO NPs), corrosion, SEM, EDX, FX, DRX…

Iron copper phosphate nanoparticles synthesis and characterization

Berrichi Amina, Bachir Redouane
University of Ain Temouchent
Corresponding author: amina.berrichi@univ-temouchent.edu.dz

Abstract:

In the preset study, we prepared copper iron phosphate nanoparticles via hydrothermal method using mild conditions as heterogeneous catalyst; which was characterized by several methods such as MET, XRD, and SEM. The characterization demonstrated that the catalyst presented nanostructured particles with size lower than 10 nm. Also, the XRD patterns exhibited a new crystalline structure. The catalyst presented high activity in the coupling of amine, aldehyde and alkyne. The same catalyst was used in the coupling AHA of amine, diiodomethane and alkyne. In addition, the stability of the catalyst was studied and leads to synthesize propargylamines derivatives with yields of 100% for six runs without loss of activity.

Natural diatomite mediateds spherically monodispersed ferrihydrite for efficient photocatalytic of textile dye

Walid Rezig

University of Sciences and the Technology of Oran Mohamed Boudiaf (USTO-MB)

Corresponding author: walidrzg@gmail.com

Abstract:

Ferrihydrite silicide is widely used to realize contact terminals of integrated circuits and is usually formed by ex-situ heating treatments in-situ reactions during sputter deposition of a ferrihydrite with SiO2 of diatomite have been investigated in this work, by means of x-ray diffraction , x-ray fluorescence , infrared spectroscopy, , scanning electron microscopy. Diatomite which will be modified by iron " the deposit of ferrihydrite on raw diatomite by FeCl2, and NaOH. Comparison of XRD results proves that raw diatomite has an irregular structure but it becomes more regular at ferrihydrite modified to obtain ferric oxides differents phases from cristallinities are: ferrihydrite , maghemite, magnetite, akaganeite,hematite, goethite, and schwertmannite. Kinetics photodegradation (photocatalytic degradation) depend a pH solution Vat Green 03 textile dye. It is more important with low pH (pH= 4).Ferrihydrite modified diatomite (DMF1) offer a great potentials for dyes eliminations and their wastewaters.

Synthesis and characterization of calcium ferrite $CaFe_2O_4$ by nitrate route

Hamza Medjadji, Maroua Benlembarek, Ali Boulaho Uache, Nassima Salhi1, Nachida Bensemmane, Mohamed Trari

Affiliation of the participant: LCPMM, University of Blida1, Algérie.

Corresponding author: hamzamedjadji1990@gmail.com

Abstract:

In this study, a Nano-spinel tetroxide, CaFe2O4, was prepared by the nitrate route. Using Ca(NO3)36H2O and Fe(NO3)39H2O as raw materials. The precursor salts were first dehydrated in a desiccator under vacuum for several days. Then, they dissolved in distilled water, and the homogeneous solution was evaporated with stirring until the solvent had completely evaporated. The obtained product was then calcined in air at 850°C. The XRD analysis of the prepared powder indicated the formation of a pure spinel phase at 850°C with an orthorhombic structure (Space Group: Pbnm, N° 62) and an average crystallite size of 31nm. It belongs to the scale of Nano-metric materials. SEM analysis showed the appearance of small grains with semi-spherical morphology. The EDX analysis detected only Ca, Fe, and O elements, thus indicating the absence of any other contaminating elements and, therefore, the high purity of the material. The XPS analysis revealed the presence of Ca2+, Fe3+, and two different oxygen species on the surface of the material. The spinel phase is recognized by the lower frequency band and higher frequency band in FTIR, where intrinsic stretching vibrations of metal, the absorption of inorganic materials compounds occurs below 1000 cm-1. The bands in the region (870-719 cm-1) attributed to O–Fe–O, Fe-OH bonds, and the peaks at 808, 636, 574, and 436 cm-1 corresponded to Ca–O and Fe–O. The Mott-Schottky analysis showed a p-type semiconductor of CaFe2O4.

ITO/GaAs contact properties for solar cells applications

Ouiza Boussoum, Fazia Bouaraba, Charles Renard, Djedjega Hatem
Affiliation of the participant: Mouloud Mammeri University of Tizi Ouzou
Corresponding author: ouiza.boussoum@ummto.dz

Abstract:
In this work, we propose to study the influence of annealing temperature and gas on the properties of ITO/GaAs contact. First, we presented the characteristics of ITO thin films, then we present the propreties of the ITO/GaAs contact that we deposited by RF sputtering and the linear Transmission Line Model (l-TLM) method was used to evaluate the ITO/GaAs contact properties The l-TLM patterns are made on n-GaAs samples, orientation (100), resistivity 10-3 Ω.cm and carrier concentration N= 2. 1018 cm-3, by laser lithography. The ITO/GaAs contact was annealed at 450°C and 500°C for different times under vacuum, ArH2 and N2 atmosphere. The ITO thin films were deposited by sputtering and show a resistivity of 10-4 Ω .cm and an average transmittance of more than 90% in the visible range. The lowest specific contact resistance of ITO/GaAs is about 1.53. 10-3 Ω.cm2 for annealing at 500°C in vacuum, 1.65. 10-3 Ω.cm2 for annealing in ArH2, and 2.36.10-4 Ω.cm2 for annealing in N2 atmosphere. The Annealing at 450°C under nitrogen atmosphere tends to be ohmic (linear), resulting in a high RSC value, and for temperatures of 500 and 550°C it decreases, with the smallest value observed at 550°C, of the order of 10-5 Ω.cm2 , and at 600°C it increases. This is the best ohmic contact between ITO and n-GaAs ever reported. These results suggest that good quality ITO has great potential to be used in the realisation of highly efficient solar cells.

Keywords: Thin films, ITO, Transparent conductor, ohmique contact, TLM method.

Effect of aging on the structural and optoelectronic properties of titanium doped zinc oxide elaborated by DC reactive magnetron sputtering

Bouaraba Fazia, Salem dalila, Boussoum Ouiza, Hatem djedjiga, Lamri Salim

Affiliation of the participant: Mouloud Mammeri University of Tizi Ouzou

Corresponding author: fazia.bouaraba@ummto.dz

Abstract:

TCO degradation is one of the main causes of aging in PV modules, this degradation is promoted by exposure to environmental stressors such as irradiance, heat and humidity, therefore understanding the phenomena of TCO degradation is essential to improve the stability and extend lifetime of the solar cells. Numerous researches focused on the synthesis and the study of Titanium doped zinc oxide properties , but in the other hand its long-term stability and degradation mechanisms of these materials has never been studied although is an essential and critical parameter for improving the lifetime performance of a material. In this study, the effect of accelerated aging upon exposure to several conditions (temperature, humidity and irradiation) in the properties of TZO thin films deposited by direct current magnetron co sputtering is investigated in order to provide a quick and direct view of the lifetime performance of a material. The results showed that annealing has a significant effect on the lifetime of TZO thin layers, so the layers annealed at 400°C has better properties than the not-annealed layers and very good fatigue resistance under accelerated aging conditions. So, annealing can be a solution to minimize aging effects and increasing the materials lifetime, to consider a wide use of these materials in photovoltaic applications.

Keywords: Transparent Conductive Oxides, TZO, Degradation, accelerated aging.

Preparation, morphological and optical characterization of Bi2O3 thin films electrodeposited on porous silicone surfaces

Lakrouf Islem, Boudinar Salem, Kellou Hamza, Amirouche Saifi, Benbrahim Nassima.

Laboratory of Physics and Chemistry of Materials (LPCM), Mouloud Mammeri University of Tizi-Ouzou

Corresponding author: islem.lakrouf@fs.ummto.dz

Abstract:

This study focuses on the electrodeposition of thin bismuth oxide films on porous silicon (SiP) surfaces prepared by chemical etching.

Electrochemical analysis by cyclic voltammetry of the kinetics of bismuth deposition highlighted the formation of a deposit on the SiP surface.

Morphological characterization by scanning electron microscopy revealed the formation of a Bi2O3 deposit in the form of discontinuous films which partially cover the porous silicon surface.

The optical characterization of the samples (Bi2O3/SiP) by UV-Vis spectrophotometry showed an evolution of the absorbance as a function of the pH of the solution.

The study of the photodegradation of BM in the presence of bismuth oxide showed a degradation rate close to 83%.

Keywords: Porous silicon, Bismuth oxide, Electrodeposition, Optical properties.

Comparative study of Metrohm 110 Screen Printed Electrode Modifications: Nickel Nanoparticles versus Nickel Tetrasulfonated Phthalocyanine for Enhanced 4-Aminophenol Detection: Elaboration and Characterization

Makhlouf Fatima Zahra, Chelaghmia mohamed lyamine,
Affoune Abed Mohamed, Makhlouf Azzedine
Laboratory of Industrial Analysis and Materials Engineering, University May 8, 1945 Guelma
Corresponding author: makhlouffatimazahra222022@gmail.com

Abstract:

Herein, we conducted a comprehensive comparison between two modified screen printed electrodes (SPEs, Metrohm 110) for the detection of 4-aminophenol (4-AP), namely the Metrohm SPE modified by poly-NiTSPc, and the Metrohm SPE modified by NiNPs. The results confirmed the successful elaboration of spherical Ni nanoparticles perfectly covering the carbon surface, with a size of 184 nm. The electrochemical behavior of 4-AP on both modified electrodes was explored via differential pulse voltammetry (DPV). The results revealed significant differences in their performances. The Metrohm SPE/Poly-NiTSPc showed an 18% increase in the oxidation current of 4-AP compared to the unmodified SPE. However, there was no notable change in the oxidation potential of 4-AP. This indicates that the Poly-NiTSPc-based modification primarily has a geometric effect on the electrode. In contrast, modification with NiNPs on the Metrohm SPE showed a significant electrocatalytic effect. We observed a 10% increase in the oxidation current of 4-AP, accompanied by a 70 mV decrease in the oxidation potential.

Keywords: Ni nanoparticles, Nickel Tetrasulfonated Phthalocyanine, Electrochemical sensor, 4-aminophenol.

Iron copper phosphate nanoparticles: Synthesis and characterization

Berrichi Amina, Bachir Redouane
University of Ain Temouchent
Corresponding author: amina.berrichi@univ-temouchent.edu.dz

Abstract:
Phosphate material have a wide range of applications such as fluorescent materials where fluorescent lanthanide orthophosphate were used and it shown a fluorescent properties during their internalization into human umbilical vein endothelial cell. In addition, it has been considered as ceramic materials with high magnetic and electrochemical properties. Since the calcium phosphate nanoparticles utilization in biological, therapeutic and bio-medicinal fields such as treatment of cancers, caries inhibition, researchers decrease their researches by using other metals and modification of phosphate materials. For example cobalt phosphate nanoparticles, modified this one by Nickel, and Zirconium phosphate nanoparticles which are used as electro-catalyst for water treatment, dyes removal and treatment of cancers . Several methods were used to synthesize phosphate material, such as precipitation, co-precipitation, impregnation, deposition and others, and hydrothermal rout. This later can be lead to different shape and structure. In this study, we prepared iron copper phosphate nanoparticles (FeCuP) using hydrothermal rout, during preparation several conditions were used modifying the urea amount. So, different structures were achieved. The material was characterized by SEM, EDX, UV-Vis and XRD. The material was used as catalyst for synthesis of propargylamines. The nanoparticles catalyst was reused with high activity and stability.

Key words: FeCuP, nanoparticles, phosphate material, minerals

Microscopic Insights into Failure Mechanisms and mechanical properties of a PLA Biocomposite with Natural Fiber Reinforcement

Benabderazag Khalil, Guebailia Moussa, Belouadah Zouheyr
Ouargla University
Corresponding author: khalilstts@gmail.com

Abstract:
This study investigates the fracture morphology of a biocomposite composed of a PLA matrix and Lygeum spartum L. fiber reinforcements. Scanning electron microscopy (SEM) was employed to analyze the cross-section of the fractured surface. SEM images revealed the fiber distribution within the matrix and variations in fiber structure, including the presence of both bulk fiber formations and individual elementary fibers. Crucially, the images also displayed micro and nanoscale marks on the fibers. These marks are indicative of failure mechanisms under stress, such as matrix cracking, fiber pullout, and fiber debonding. This detailed morphological analysis provides valuable insights into the biocomposite's behavior and deformation mechanisms under applied stress.

Advancements in CZTS Solar Cell Technology: Properties and Fabrication Processes

Belaid Ibtissem, Bellal Tahar, Tala Ighil Razika, Toubane Mahdia
Affiliation of the participant: ENS Kouba
Corresponding author: ibtissem.belaid14@g.ens-kouba.dz

Abstract:
CZTS is composed of abundant and non-toxic elements, making it environmentally friendly and cost-effective compared to materials like CdTe and (CIGS. Additionally, CZTS has a direct bandgap suitable for solar energy conversion, allowing for efficient absorption of sunlight across a wide spectral range. In terms of its fabrication, the process of CZTS layer deposition involves several key steps. It begins with the preparation of precursor materials, including copper, zinc, tin, and sulfur salts, which are mixed in appropriate proportions to form a homogeneous solution. This solution is then deposited onto a substrate using techniques such as spin-coating, sputtering, or evaporation. Following deposition, the CZTS layer undergoes a thermal annealing process to promote crystallization and enhance its electrical properties. Annealing can be performed in controlled atmospheres to optimize crystalline growth conditions and ensure uniformity across the layer. Post-deposition treatments may also be applied to further improve the quality and performance of the CZTS layer. These treatments can include doping to adjust electrical properties, surface passivation to reduce recombination losses, and characterization techniques to evaluate the composition, structure, and optoelectronic properties of the layer.In summary, CZTS possesses advantageous properties for solar cell applications, including abundance, non-toxicity, and suitable bandgap. Its fabrication involves precise control of precursor materials, deposition techniques, and post-deposition treatments to achieve high-quality CZTS layers for efficient solar energy conversion.

Structural, morphological, optical and electrochemical properties of Cu2O nanoparticles and Cu2O nanostructures: Additives effect

Meriem Aloui, Halla Lahmar, Loubna Mentar
Quantum electronics laboratory, university of science and technology of Houari Boumedien, Bad ezzouar, Algeries,
Corresponding author: meriam_aloui@yahoo.fr

Abstract:
In this work, Cu2O polyhedrons with two different shapes were synthesized, using the galvanostatic electrochemical deposited method. In copper nitrate ðCuðNO3Þ2Þ and Potassium chloride (KCl) bath, the Cu2O show highly symmetric 26-facet polyhedral microcrystals with well-defined {100}, {110}, {111} crystallographic faces. While, in the presence of additive (NH4Cl), Cu2O shows 18-polyhedral with well-developed {100} and {110} faces. The two morphologies revealed p-type semiconducting behavior. Cu2O 26-facet polyhedral show a high photoelectrochemical (PEC) stability of 73.5%. Such a feature is of great importance for future water splitting applications. Furthermore, the influence of the potassium chloride (KCl) upon their structural, morphological, conduction type, and optical properties, were investigated, studying the Cu2O nanostructures electrodeposited. Cu2O thin films were prepared from copper sulfate as a precursor (CuSO4), using different concentrations of potassium chloride (KCl). Structural, optical, and morphological properties of films, which were obtained by galvanostatic mode, were observed. It was shown that the conduction type of Cu2O nanostructures does not change regardless of the KCl concentration in the electrolyte. However, chlorine ions can ameliorate the density of the donor carriers (30 times largest) and the morphologie can be totally changed when the concentration of Cl ions attends 0.1 M from nanocubes to dendrites of polyhedral shape.

The effect of NaOH concentration on (Ni60Co40)90Fe10 nanoparticles synthesized by hydrothermal method

Y. Gaci, A. Guittoum, M. Hemmous, D. Martínez-Blanco, P. Gorria, J. A. Blanco , T. Aouaroun

Affiliation of the participant: UMBB

Corresponding author: y.gaci@univ-boumerdes.dz

Abstract:

We studied the effect of changing the concentration of sodium hydroxide on the magnetic, structural and morphological properties of (Ni60Co40)90Fe10 nanopowders. These nanopowders have been synthetized using hydrothermal method. The characterization of our samples relied on X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) and vibrating sample magnetometry (VSM). We have shown the presence of a cubic face centered (cfc) phase for all samples except only one sample that showed the presence an additional hcp phase. The lattice parameters of all samples increase with increasing NaOH concentration. Also, the grains size changes with NaOH concentration change to reach a minimum value of 22 nm for the sample synthetized with 3g of NaOH content. The saturation magnetization, Ms, and the coercivity, Hc calculated from Hysteresis curves, have been investigated. The values of Ms, and Hc are found to have minimum values for the same sample synthetized with 3g of NaOH.

Elaboration and characterization of $Li_2B_4O_7$: Eu^{3+}, Sm^{3+} glass

R. Belhoucif [1, 2, 3], A. L. Benmaiza [1,] and M. Medjbour [2]

[1] *Laboratory of Quantum Electronics, Faculty of Physics, USTHB, BP 32, 16111, Algiera.*

[2] *Department of physics, Faculty of Sciences, UMBB Boumerdes, Algeria.*

[3] *Coating, Materials and Environment Laboratory, UMBB, Boumerdes, Algeria.*

Corresponding author: abdelkader.benmaiza@gmail.com

Abstract:

Lithium borate-based materials find applications in diverse fields such as scintillators, thermoluminescence dosimeters, γ and neutron detectors, lasers, second harmonic generation, optoelectronic devices, supercapacitors, energy storage, photonic devices...etc. LTB's properties, coupled with its ability to accommodate trivalent lanthanides, makes it a promising candidate for various spectroscopic and luminescence applications.

In this work, Eu^{3+} and Sm^{3+} co-doped $Li_2B_4O_7$ glass was synthesized by conventional melt quenching method. The amorphous nature of the glass sample was confirmed by XRD spectrum. The optical band gap (Eg=3.23 eV) and refractive index (n=2.3) were performed from the diffuse reflectance spectra, by plotting the KubelkaeMunk remission function. Luminescence spectra and decay kinetic of the prepared glass excited at 405 nm were recorded and discussed.

Key words: tetraborate, scintillators, thermoluminescence, laser, supercapacitors, photonic devices, absorption, KubelkaeMunk, luminescence.

Effect of Aqueous Solution pH on the Photocatalytic Performance of ZnO Nanoparticles on Rhodamine B dye

Mahdia Toubane1, Fares Chabira [1], Asma Bessaad [2], Razika Tala-Ighil[1], Fayrouz Benhaoua, Lamri Younes[1] and Messaid Bachir Eddine[1]

[1]*URMPE Unite, UMBB University, 35000 Boumerdes, Algeria*

[2]*Benyoucef benkhda Université, Alger 1*

Corresponding author: m.toubane@univ-boumerdes.dz

Abstract:

The ZnO nanoparticulcatalystpreparedusing UV irradiation was extensively characterized using several techniques including, infrared spectroscopy (FTIR) and X-ray diffraction (XRD) and Raman spectroscopy. We chose Rhodamine (RhB) dye as a model contaminant in order to investigateits Photocatalytic activityunder UV light irradiation. The effect of pH on degradation réaction wes also investigated. The structural analysis of the oxide nanoparticles (ZnO) shows a Wurtzite structure withpreferred orientation (101). The Raman spectroscopy confirms that the ZnO nanoparticles crystallizef rom the hexagonal Wurtzite structure by the presence of E2 (low) and E2 (high) mode. The FTIR spectra show absorption lines located at wave numbers corresponding to vibrational modes between constituent atoms of the compound. RhB photocatalytic effciencyishighest in acid medium and minimal in basic medium.

Keywords: ZnO nanoparticul, thermal treatment, XRD, Raman, FTIR, pH, Photodegradation of RhB.

Effect of Fe/Al ratio on the hyperfine and magnétiques properties of three-dimensional nanostructred Iron-Aluminum alloys

Nadia Boukherroub [1], Abderrahim Guittoum [2] and Messaoud Hemmous[2]

[1] *UR-MPE, M'hamed Bougara University, Boumerdes, 35000, Algeria*

[2] *Nuclear Research Centre of Algiers, 02 Bd Frantz Fanon, BP 399 Alger-Gare, Algiers, Algeria*

Corresponding author: nadia.boukerroub@yahoo.fr

Abstract:

In the present work, we study the effect of Fe/Al ratio on the hyperfine and magnétiques properties of nanocrystalline Fe_xAl_{100-x} alloys prepared by mechanical alloying process. These properties were investigated by means of Mössbauer spectroscopy and vibrating sample magnetometer (VSM) measurements at room temperature. It was found that the spectra of samples with Fe:Al ratio of 80:20, 75:25, and 70:30 exhibits a fully ferromagnetic behavior. However, the spectrum of the sample with Fe:Al ratio of 60:40 is composed of a sextet (ferromagnetic phase) and a weak paramagnetic singlet. Also, the VSM test results indicated that by decreasing the Fe/Al the saturation magnetization (M_s) decreased and coercivity (H_c) increased. All the results will be correlated and discussed.

Keywords: Nanostructured FeAl powders, mechanical alloying, Mössbauer spectroscopy and hysteresis loops.

Elaboration and morphological study of iron oxide nanostructure

S. Lamrani1, R. Belhoucif[1], M. Ifires [2]

[1] *Laboratoire Revêtement, Matériaux et Environnement, UMBB, Boumerdes, Algeria*

[2] *Division Technologies Emergentes des Semis Conducteurs pour l'Energétique, Centre de Recherche en technologie des Semi-Conducteurs pour l'énergétique, 2 Bd Frantz Fanon, BP 140 les 7 merveilles, Algiers, Algeria*

Corresponding author: sa.lamrani@univ-boumerdes.dz

Abstract

In this work we report the preparation of iron oxide films deposited on a nanostructured silicon and their morphological characterization. The nanostructured template was elaborated usingAg assisted electroless chemical etching at room temperature. Iron thin films were elaborated by electrochemical road, using cyclic voltammetry and chronoamperometry methods. Three electrochemical cell, (Ag/AgCl) reference electrode, and a nanostructured n-Si (100) work electrode were used during the deposition process. The obtained cyclic voltammetry (CV) exhibits cathodic and anodic peaks, situated at -1.02V/ (Ag / AgCl) and 0.2V/ (Ag/AgCl) respectively. The obtained Fe films were oxidized by used thermal annealing at 500 °C in an oxygen atmosphere. From SEM micrographs, we evidenced that the α-Fe_2O_3 hematite phase deposits grow both on the surface and into the silicon nanostructure substrate.All these results will be correlated and discussed.

Keywords: Electrochemistry, Iron oxide, SEM.

Exploring the Influence of PVP 360 on the Properties of Hydrothermally Synthesized ZnO Nanoparticles for Photocatalysis

Fares Chabira [1,2], MahdiaToubane[1,2] and Razika Tal-Ighil[2,3]

[1]*Physics Department,Faculty of Sciences, University M`Hamed bougara, 35000 Boumerdes,Algeria*

[2]*URMPE Unit, M'hamed bougara University, 35000 Boumerdes, Algeria*

[3]*Institute of Electrical and Electronic Engineering, M'hamedBougara University, 35000*

Corresponding author: f.chabira@univ-boumerdes.dz

Abstract:

Zinc oxide is an inorganic compound and usually appears as a white powder. It also called a multifunctional material because of to its unique physical and chemical properties. Zinc oxide nanoparticles were successfully synthesized by a hydrothermal method using a solution containing zinc nitrate hexahydrate, and polyvinylpyrrolidone with different percentages. Different compositions of zinc oxides nano composites were characterized using X-ray diffractometer, Fourier-transform infrared spectroscopy. X-ray diffraction analysis indicates the formation of pure high-quality ZnO phase with a hexagonal Wurtzite-type structure.The FT-IR analysis reveals a prominent peak at 600 cm^{-1} typical characteristic of Zn–O bond. Photocatalytic tests show that all nanopowders significantly degrade the malachite green under ultraviolet light.This research Focuses on the potential of ZnO nanoparticles as a sustainable method for various applications, especially in environmental cleanup efforts such as purifying water fromorganic/inorganic compounds.

Keywords: Hydrothermal, PVP360, ZnOnanoparticles,Photocatalytic.

Microwave-assisted synthesis of metal oxide nanoparticles: Comparative study with conventional approaches

Imane Djouabi [1], Nadia Boukherroub[2], Mahdia Toubane[2] and Meriem Djanette Blizak[3]

[1]*Higher Normal School of Kouba, Physical Science Department,B.P N°92 16308 Vieux-Kouba–Algeirs, Algeria,*
[2]*UR-MPE, M'hamed Bougara University, Boumerdes 35000, Algeria ,*
[3]*L-BMAB, M'hamed Bougara University, Boumerdes 35000, Algeria ,*

Abstract:
Metal oxide nanoparticles have been widely used in recent years for a variety of purposes, including solar cells, photocatalytic degradation, sensors, antibacterial qualities, and supercapacitors. Transition metal oxides (NiO, ZnO, TiO_2 , SnO_2, CuO, $\gamma - Fe_2O_3$, ...etc.) are the most desirable of all the metal oxides because of their exceptional electrical, magnetic, and catalytic properties, which allow them to be used in a variety of applications. In order to create transition metal oxide nanoparticles for a range of uses, a number of processes have recently been used, including sol-gel, hydrothermal, microemulsion, chemical precipitation, the green synthesis method, and microwave-assisted approaches. Because microwave-assisted procedures are more economical, quicker, cleaner, more energy-efficient, more controlled, and less time-consuming than traditional wet chemical approaches, they have gained prominence in the field of synthetic technology. In this article, they have gained prominence in the field of synthetic technology. A comparison with conventional approaches is also conducted, concentrating on key aspects such as particle size, structure, morphology, optical property, photodegradation, and supercapacitors.

Keywords: Nanomaterial, Metal oxide, Microwave synthesis.

Effect of the sol-gel and hydrothermal preparation method on the physicochemical and catalytic properties of CuAlOx material. application in the reduction of benzaldehyde reaction.

Haddad Naima, Adel Saadi, Axel Löfberg

Affiliation of the participant: Laboratoire de gaz naturel, Faculté de Chimie, USTHB

Corresponding author: akrour_naima@hotmail.com

Abstract:

The choice of synthesis method significantly impacts the physicochemical properties of materials, even with identical compositions, making it crucial for precise catalytic applications. Parameters such as crystallinity, homogeneity, morphology, and dispersion can be altered accordingly.

In this regard, We synthesized bimetallic oxide Cu-Al-O (Cu/Al=1) using the sol-gel method (designated CuAl-SG) and compared it with the hydrothermal system (CuAl-Hyd). Both systems were thermally treated under N2 at 500°C and characterized using XRD, BET-BJH, and SEM techniques. Catalytic activity was assessed in the reduction of benzaldehyde within the 150-200°C temperature range. The XRD comparison of CuAl-Hyd and CuAl-SG systems reveals the influence of the preparation method on the structural properties of Cu-Al-O. While the hydrothermal system forms CuO and Al2O3 oxides, the sol-gel method produces CuAlO2 with a hexagonal delafossite structure. The preparation method also affects the textural properties of CuAl. Porosity results show a significant difference, with the specific surface area of CuAl-Hyd being 80% larger than CuAl-SG (106 m2/g vs. 22 m2/g). The BJH analysis indicates a more homogeneous pore distribution in the sol-gel system, characterized by two peaks representing different pore sizes. SEM imaging highlights distinct morphologies between CuAl-SG and CuAl-Hyd, with the former displaying uniformity and particle agglomeration. Additionally, CuAl-

Hyd exhibits smaller particles with uniform size distribution and lower crystallization degree.

CuAl-SG demonstrates superior reactivity in benzaldehyde reduction, with enhanced conversion (3% to 28% and 54% to 79%) and selectivity towards benzyl alcohol (0% to 46% and 0% to 34%) at 150 and 200°C. The copper oxidation state (+I) in $CuAlO_2$ favors the activity of CuAl-SG. Furthermore, the sol-gel system's homogeneous pore distribution and small pore volume with a high average diameter may facilitate benzylate species desorption, enhancing selectivity towards benzyl alcohol.

Study of photo-conversion performance of carbon-based perovskite solar cells working on high temperature

Mohammed El Said Sarhani, Tahar Dahame
Université Amar Telidji de Laghouat
Corresponding author: m.sarhani@lagh-univ.dz

Abstract:
In this research, a carbon-based perovskite solar cell (C-PSC) structure was designed to obtain a better photo-conversion performance and a more stable device. Here, several perovskite materials, such as ABI3 (A= MA, FA, Cs, and B=Pb, Ge, Sn) were used as an active absorber layer. The impacts of perovskite layer thickness, deep defect density, and device working temperature on the cell performance were studied. Furthermore, we investigated current-voltage (J-V) hysteresis phenomena in perovskite-based solar cells using defect models. The results show that FASnI3 is the most efficient carbon-based solar cell, with a power conversion efficiency (PCE) of 24.11%. This research paves the way for metal iodide to be used as an active layer for C-PSC to produce more reliable and efficient solar cells.

Investigation of the lead-free double perovskite K2AgSbI6 for optoelectronic and thermoelectric applications

Merrad amel, Halima Bouchenafa, Boucif Benichou
Department of Physics, Faculty of Exact Sciences and Informatics, Hassiba Benbouali University of Chlef
Corresponding author: a.merrad@univ-chlef.dz

Abstract:
In this work, theoretical investigations of the structural, elastic, optoelectronic, and thermoelectric properties of K2AgSbI6 have been carried out. The indirect band gaps of 0.874 eV and 0.331 eV were calculated using the TB-mBJ potential and the PBE-GGA approximation. Moreover, the obtained elastic constants C11, C12, and C44 ensure the mechanical stability and ductility nature of the studied alloy. The findings of the optical properties suggest that K2AgSbI6 exhibits a high absorption coefficient and low optical reflectivity in the visible and ultraviolet spectra. In addition, the Seebeck coefficient, power factor, and figure of merit were calculated using the BoltzTrap code. The negative temperature coefficient of resistivity also supports the semiconductor nature of this compound. The high electrical conductivity, low thermal conductivity, positive Seebeck coefficient, and optimum figure of merit make this compound suitable for thermoelectric applications. Finally, the reported results should serve as a stimulus for future experimental and theoretical investigations.

Keywords: Double perovskite, Elastic constants, Structural properties, Thermoelectric properties, Optoelectronic properties.

Impact of Rare Earth Element Doping on Enhancing the Photoactivity of the Perovskite KNbO3 for Hydrogen Production Under Visible Light

Mekersi Romaissa , Boumaza Souhila , Trari Mohamed
Laboratory of Chemistry of Natural Gas Faculty of chemistry,USTHB, BP 32 El Alia, Bab Ezzouar, 16111 Algiers, Algeria
Corresponding author: mekersi.romaissa1997@gmail.com

Abstract:
Humanity faces pressing challenges in energy shortages and environmental pollution. Hydrogen, as a clean energy carrier, is a promising solution, particularly through photocatalytic water splitting. Semiconductors like KNbO3 play a crucial role, but their wide band gap limits efficiency in the visible spectrum. To overcome this, doping semiconductors with rare earth elements is essential, modifying their properties for better performance. Our research explores these mechanisms, aiming to enhance solar energy use for hydrogen production. A rare earth-doped KNbO3 photocatalyst was synthesized using the nitric combustion method and subjected to treatment at 700°C. To thoroughly characterize this oxide, multiple physico-chemical techniques were employed: X-ray Diffraction (XRD) was utilized to discern its crystalline structure, X-ray Photoelectron Spectroscopy (XPS) provided insights into the surface composition and elements oxidation state, Scanning Electron Microscopy (SEM) allowed for detailed examination of the morphology and determination of grains size, the diffuse reflectance was employed to analyze its optical properties. These comprehensive characterizations aimed to validate the successful synthesis and assess the catalyst's potential for hydrogen production under visible light conditions.

Efficiency enhancement of organic solar cells with different concentrations in volume ration of Ag nanoparticles incorporated into the PEDOT:PSS layer

Salem Dalila , Bouaraba Fazia, Benseba Ghalia, Hatem Djedjiga and Jean-Michel Nunzi

Mouloud Mammeri university of Tizi Ouzou

Corresponding author: dalila.salem@ummto.dz

Abstract:

In this study, Different concentrations in volume ration of silver nanoparticles (Ag NPs) with size 10 nm have been introduced into poly-(3,4 ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS) of inverted organic solar cells (OSCs) with a glass/ITO/ZnO/P3HT:PCBM/ PEDOT:PSS/Ag structure. Optical and electrical characteristics were measured using the UV-Visible and current-voltage characteristic J(V). We observed that the conversion efficiency of the solar cells improved to 2.18% compared with 1.40% for the cell without Ag NPs, when the concentration of Ag NPs in PEDOT:PSS was 20 % vol. But the addition of Ag NPs at 30% vol concentration caused a drop in Jcc, reducing efficiency to 1.90 %. The improvement in device performance is attributable to the electrical enhancement of the PEDOT:PSS layers by the presence of Ag NPs. Our results show an increase in barrier height associated with NPs addition as supported by the varying values of the ideality factors and series resistances. Absorption spectrums of the active layers have no clear contribution to optical absorption improvement in the devices.

Keywords: Inverted OSCs, PEDOT:PSS layer, silver nanoparticles, volume ratios NPs.

Synthesis, characterization and evaluation of the photocatalytic activity of iron oxide doped with zinc nanomaterials

Doumi Bouthaina, Bendeddouche Choukry Kamel, Adjdir Mehdi
Laboratoire de synthèse organique appliquée université Oran 1
Corresponding author: doumibouthaina@gmail.com

Abstract
This study presents the synthesis and characterization of composite materials comprising Iron-based layered double hydroxides (Fe-LDHs) generated through the co-precipitation method, along with their corresponding calcined Iron-based layered double oxides (Fe-LDO). These composites aim to effectively eliminate the cationic dye "Methylene Blue" (MB) and exhibit antibacterial properties against both Gram-positive and Gram-negative bacteria. Various characterization techniques, including X-ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR), were applied to examine the synthesized nanocomposites. XRD analysis confirmed the presence of both hydrotalcite-like and LDO phases within the nanocomposites. The adsorption behavior of MB dye was studied by analyzing different physicochemical variables.The results revealed that Fe-LDHs and Fe-LDO demonstrated notable adsorption capacities for MB dye, achieving a maximum removal efficiency of 85% within 30 minutes. Additionally, the findings underscored the inhibitory effects of Fe-LDHs and Fe-LDO on bacterial growth at a dosage of 10 mg, indicating the promising potential of both nanocomposites as antibacterial agents.

Keywords: Composite materials, Iron-based layered double hydroxides (Fe-LDHs)Co-precipitation method, Calcined Iron-based layered double oxides (Fe-LDO), Cationic dye, Antibacterial properties.

Study of photo-conversion performance of carbon-based perovskite solar cells using SCAPS-1D simulator

Mohammed ElSaid Sarhani , Tahar Dahame
University of Laghouat
Corresponding author: m.sarhani@lagh-univ.dz

Abstract:

In this research, a carbon-based solar cell structure is designed to obtain a better photo-conversion performance and a more stable device. Here, several perovskite materials, such as ABI3 (A= MA, FA, Cs, and B=Pb, Ge, Sn) are used as an active absorber layer. The impact of perovskite thickness, deep defect density and device working temperature on the cell performance are studied. Furthermore, we investigate J-V hysteresis phenomena in perovskite-based solar cells using defect models. The results show that FASnI3 is the highest efficient carbon-based solar cell, with an efficiency of 24.11%. This research paves the way for metal iodide to be used as an active layer for C-PSC to produce more reliable and efficient solar cells.

ZnO Nanoparticle Synthesis via Cold Plasma: Investigation of Structural and Optical Characteristics, and Photodegradation of Methylene Blue dye

MESSAI Ridha, Ferhat Mohamed Fouad, Bounedjar Nourelhouda
university of el-oued
Corresponding author: messai-ridha@univ-eloued.dz

Abstract:
In this investigation, non-thermal plasma (NTP) was utilized as a method for synthesizing zinc oxide (ZnO) nanoparticles (NPs). This technique is renowned for its capability to produce NPs with precise characteristics and is distinguished for its environmentally friendly attributes. Comprehensive characterization of the synthesized NPs was undertaken employing various analytical methods, providing valuable insights.
The analysis unveiled that the ZnO NPs exhibited a hexagonal wurtzite crystal structure, with an average particle size of 25 nm. Scanning electron microscopy (SEM) observations revealed particles of varied sizes and agglomerations, showcasing pseudo-spherical and non-uniform hexagonal shapes. Additionally, UV-visible spectroscopy measurements indicated a distinct absorption peak at 368 nm, corresponding to a bandgap energy of 3.30 eV.
To evaluate the photocatalytic efficacy of the ZnO NPs, their capability to degrade Methylene Blue dye under UV irradiation was assessed. Remarkably, the NPs demonstrated a satisfactory photodegradation efficiency of 41% within a 90-minute duration.
This investigation emphasizes the potential of non-thermal plasma for synthesizing ZnO nanoparticles possessing exceptional properties, without necessitating additional chemicals. These environmentally benign nanoparticles, hold significant promise for various photocatalytic applications.

Nano-Encapsulated Phase Change Materials (ePCMs) for Solar-Thermal Applications

Farida Iachachene, Hanane Cheradi, Louiza Achab, Malika Kabache
Energy, Mechanics and Engineering Laboratory (LEMI), M'hammed Bougara University, Boumerdes, Algeria
Corresponding author: f.iachachene@univ-boumerdes.dz

Abstract:
Phase Change Materials (PCMs) have gained significant attention for their remarkable capacity to store and release thermal energy during phase transitions. This study delves into the exploration of nano-encapsulated phase-change materials (ePCMs) and their potential to revolutionize the solar-thermal industry. The seamless integration of ePCMs from research to market necessitates a comprehensive understanding of their application domains, a focal point of this investigation. Emphasizing the application of nano-scale ePCMs, this study underscores their efficacy in latent heat storage with solid-liquid PCM cores and their use of surface-engineered shells to mitigate solar radiation. By presenting specific examples of successful applications of ePCMs in solar-thermal systems and integrating relevant research findings and experimental data, this study aims to elucidate the transformative potential of ePCMs in the solar-thermal industry.

The use of polymer-based nanofluids in drilling fluids: Perspectives and Applications

S. Remli[1], K. Benyounes[2], A. Benmounah[2]

[1]*Unité de Recherche Matériaux, Procédés et Environnement, Université M'hamed Bouguara Boumerdes, 35000, Algeria*

[2]*Laboratoire Génie Physique des Hydrocarbures, Université M'hamed Bouguara Boumerdes, 35000, Algeria*

Corresponding author: s.remli@univ-boumerdes.dz

Abstract:

Polymer-based nanofluids are colloidal suspensions composed of nanometric particles dispersed in a base fluid, such as water or oil. These nanofluids have unique properties that can be exploited in a variety of industrial applications, including the oil and gas industry. This review focuses on the use of polymer-based nanofluids in drilling fluids, which are liquids used to facilitate the process of drilling oil and gas wells. Nanofluids offer several potential advantages over conventional drilling fluids, such as improved drilling performance, reduced fluid loss, and stabilization of geological formations. We explore the unique properties of polymeric nanomaterials, including their thermal stability, friction-reducing ability and effectiveness in controlling circulation losses. In addition, we discuss the technical challenges and opportunities associated with integrating polymeric nanofluids into current drilling practices. In the end, this article highlights the promising potential of polymer-based nanofluids to improve operational efficiency, reduce costs and minimize the environmental footprint of the drilling industry.

Keywords: Polymeric nanofluids, Drilling fluids, Rheological properties, Thermal stability, Cooling capacity, Lubrication, Drilling performance.

Analyzing the Evolution of Nickel Oxide Nanoparticles in Environmental Research

Missouni hayet[1], Blizak Meriem Djanette[2] , Toubal Souheyla [2]

[1]*LN-corps SM, Higher Normal School of Kouba Echeikh Mohamed Elbachir Elibrahimi, Vieux-Kouba, Algeria.*

[2]*Bioinformatics, Applied Microbiology and Biomolecules Research Laboratory (BMAB), University M'Hamad Bougar of Boumerdes, Algeria*

Corresponding author: hayet.missouni@g.ens-kouba.dz

Abstract:

In terms of the environment, the use of nanomaterials is envisaged for the reduction of pollutant emissions, the treatment of effluents in particular by photocatalysis and the purification of gases, the production of ultra-pure water from sea water, wastewater and air treatment. Different treatment methods are developed to meet the daily needs of the most used people settling, filtration, adsorption… Due to their dual-action mechanism, which combines adsorption and photocatalytic activity, NiO-NPs are highly effective photocatalysts against dye pollutants in the field of environmental restoration. First, NiO NPs participate in adsorption, serving as molecular magnets to attract dye molecules to their surface and provide close contact that is necessary for the photocatalytic destruction that follows. When the activated NiO NPs come into contact with light, they release reactive species such hydroxyl radicals that effectively break down the adsorbed dye molecules. Their effectiveness in water treatment, air pollution control, and energy conversion has displayed significant potential, primarily due to their ability to generate reactive oxygen species and maintain stability. The results of these studies indicate that NiO nanoparticles possess favorable photocatalytic characteristics and can potentially be used as an effective solution for removing dyes from water, with a removal efficiency of up to 99.6% for Methylene blue (MB) dye. In this context, we focus on the remarkable surge in research

dedicated to metal oxide nanoparticles, in particular nickel oxide nanoparticles, evident in the consistent growth of annual publications.

Multifunctionality of Zinc Oxide Nanoparticles: Environmental and sustainable energy

Bessaad Asma[1] and Kouachi Raïd[2]

[1] *Alger 1, benyoucefbenkhda, university , Algeria*

[2]*Department of Physics, UMBB University, 35000 Boumerdes, Algeria*

Abstract :

The sharp increase of organic pollutants across diverse environmental mediums as well as the escalating global demand for clean and sustainable energy sources both highlight the need for innovative solutions. Nanomaterials can act as photocatalysts for environmental remediation by causing the degradation of organic pollutants in water and air, converting them into harmless byproducts. Nanomaterials can also act as photocatalysts to address the challenges in sustainable energy, through photocatalytic water splitting for hydrogen production. In this work, we have explored the potential of Zinc Oxide nanomaterial as a photocatalyst for the degradation of organic pollutants and production of hydrogen gas. The choice of Zinc Oxide is due to its wide range of interesting and useful properties, such as a high photocatalytic activity, wide bandgap for light absorption, physical and chemical properties, no toxicity, water insolubility, biocompatibility, chemical stability, abundance, and low cost. Additionally, the study investigates the feasibility of incorporating Zinc Oxide into self-cleaning surface applications, aiming to enhance its capability in multi-functionalities for environmental and industrial surfaces.

Keywords: Zinc Oxide Nanoparticles,photocatalysts, hydrogen production, self-cleaning surface.

NiO thin films synthesized with Lemon juice and their photocatalytic activities

Imane Djouabi[1], Mahdia Toubane[2] ,Nadia Boukherroub[2] and Meriem Djanette Blizak[3]

[1]*Higher Normal School of Kouba, Algeirs, Algeria,*

[2]*UR-MPE, M'hamed Bougara University, Boumerdes 35000, Algeria ,*

[3]*L-BMAB, M'hamed Bougara University, Boumerdes 35000, Algeria,*

Corresponding author: imane.djouabi@g.ens-kouba.dz

Abstract:

This research presents a green chemistry approach for the synthesis of NiO thin films using plant extract as reducing and stabilizing agents. Lemon juice was utilized for the reduction of nickel ions. $Ni(NO_3)_2, 4H_2O$was used as the precursor, distilled water served as the solvent and lemon juice with some drops of DEA as stabilizer. In the green synthesis of NiO,1.4933 g of the $(Ni(NO_3)_2, 4H_2O)$ precursor ıs dıssolved ın 25ml of distilled water then 5 ml of the lemon juice was added drop by drop, the synthesis was conducted under ambient conditions. Finally, a clear homogeneous solution was obtained. Glass substrates were washed with a liquid detergent, rinsed with distilled water .They were then ultrasonically cleaned and rinsed in ethanol and distilled water for 15 min at 60 °C. The precursor solutions were deposited by dip-coating technique, consisting in the substrate immersion and nits withdrawn from the Teflon pot that contains the sol. The withdrawal speed was fixed at $11 mm.s^{-1}$. The films were then dried at 400 °C for 10 min to remove solvent and residual organics. This process was repeated 4 times to increase the film thickness. Finally, the as-deposited NiO thin films were annealed at 500 °C for 40 min to improve the film's phase formation, crystallinity and density.

Keywords: *NiO thin* films, greensynthesis, lemon juice.

The Choice of Hole and Electron Transport Materials and Impact of Temperature on Performance of Perovskite Solar Cells

Ourahmoun Ourida

University of Mouloud Mammeri of Tizi-Ouzou
Corresponding author: ourida.ourahmoun@ummto.dz

Abstract:
The hybrid metal halide perovskites exhibit attractive optoelectronic properties, such as high absorption coefficient, ambipolar charge carrier mobility, longer carrier lifetime and diffusion length, which make them a favorable material for efficient solar energy harvesting. Lead toxicity has been reported to impact the ecosystem and human health during the manufacturing, use, and recycling phases. As a result, replacing lead with a non-toxic element and organic components with inorganic ones while improving stability is an excellent way to progress toward commercialisation. Charge transporting materials are essential for fabricating stable and efficient perovskite solar cells. The low-cost processing, better solubility, efficient charge mobility, and better stability of organic compounds are some properties for their utilization as charge transport materials in perovskite solar cells. Nanoparticules of transparent oxides : titanium oxide (TiO2) and zinc oxide (ZnO) are used as electron transport layers. The electrical parameters of the cells depend on temperature and light intensity. To improve stability of perovskite solar cells, solution are proposed such as defect passivation of the perovskite layer using quantum dots, encapsulation of cells is used to protect cells against diffusion of water and oxygene, and tandem structures are used to improve efficiency.

Impact of the interconnect material on the total power dissipation of the CMOS inverter at 7 nm node technology

Lazzaz Abdelaziz, Beladam Fatiha, Bousbahi Khaled, Ghamnia Mustapha

LSMC, Université d'Oran1

Corresponding author: lazzaz.abdelaziz@gmail.com

Abstract:

An interconnect material is a thin film of conducting material that provides electrical connection between two circuits. At the ultra-small node technology scaling, Fin FET devices are promising alternative solutions to overcome the Short Channel Effect (SCE), decreasing the tunneling current and in order to have a faster CMOS circuit. The most common interconnect used in Ultra-Large-Scale Integration (ULSI) is Aluminum because it forms good ohmic contacts with Silicon, however at this nano-scaling technology, electromigration takes place. In nanoscale devices, Copper, is also another interconnect material because it has a higher conductivity. At the 7 nm node technology, power dissipation and time delay, both increases using Copper as the interconnect material. The International Roadmap for Devices and Systems (IRDS-2023) states that Ruthenium (Ru) and Low dielectric constant oxide (SiCOH) also, provide good interconnects for this technology. In this simulation, we present the impact of different interconnect materials in time delay, power dissipation, and power delay product (PDP) of the CMOS inverter at 7 nm node technology using FinFET devices. The novelty of this paper is to present three successors interconnect materials to copper and these are SiCOH, Ru and CNT because it has a minimum time delay and a minimum PDP.

Keyswords: FinFET, CMOS, Interconnect materials, Power dissipation.

PH and thermo-responsive polymeric sytem in drug delivery

Derbali Abir[1,2], Bouzid Djallel[1,2]

[1]*National Polytechnic School of Constantine, BP 75, A, Novel ville RP Constantine, Algeria*

[2]*Laboratory of Process Engineering for Sustainable Development and Health Products, BP 75, A, Nouvelle Ville RP, Constantine, Algeria*

Corresponding author: abirderbali19@gmail.com

Abstract:

In this work, the development of pH-thermo-responsive double network, with hydrophilic properties is proposed, nanoparticles are developed by the combination of two intelligent biodegradable polymers, the used method based on the copolymerization of Poly (acrylic acid) and chitosan. The influence of the acrylic acid concentration and the crosslinker on the characteristics of formulated nanoparticles have been investigated. Particle size, Zeta potential and size distribution analysis revealed that nanoparticles had a size less than 100 nm, with zeta potential about (-29.7mV) and narrow size distribution. Furthermore, the developed system showed a high encapsulation efficiency about 90%. The swelling behaviors of CS-g-PAA nanoparticles have been studied, Chitosan-g-Poly (acrylic acid) nanoparticles proved pH-thermosensitive characteristics. that makes them an interesting system for control drug release. The swelling of nanoparticles was explained according to their structures. Results revealed that swelling behaviors were affected by the crosslinker and acrylic acid concentrations.

Keywords: Chitosan, Drug delivery system, Poly (acrylic acid), pH-Thermo-responsive nanoparticles.

Green synthesis and characterization of silver Nanoparticless using aqueous extract of medicinal Plant

Azzouz Abdelhak, Fekih Nadia, Bledjilali Mohamed, Belhadj Bouchaib
Ain Temouchent university
Corresponding author: abdelhak.azzouz@univ-temouchent.edu.dz

Abstract:
Usually, nanoparticles can be synthesized by various physicochemical processes such as vapor deposition and chemical reduction. The chemicals used in these syntheses are often toxic, expensive, and not environmentally friendly.
The objective of our work is based on a synthesis of metal and oxide nanoparticles by a method that is simple, fast, and environmentally friendly, and safe for the operator. For this, we have chosen to prepare silver nanoparticles in aqueous dispersion using the aqueous extract of a medicinal plant. After we prepared the nanoparticles using a silver nitrate solution and the medicinal plant extract, we studied the effect of some factors on these particles, represented by temperature and the variation in concentrations and the pH of the solution. We obtained some results through this. Through these experiments, it became clear to us that the suitable conditions for the synthesis
of nanoparticles are represented in certain concentrations and a temperature of about 60 degrees Celsius, in an alkaline medium with a pH of 11.

Key words : Nanoparticules , medicinal plant , extraction, silver nitra"

Green synthesis of iron oxide nanoparticles and biological activities: state of the art

Toubal Souheyla, El Haddad Djillali, Missouni Hayet, Sadaoui Nesrine, Blizak Merièm Djanette

Bioinformatics, Applied Microbiology and Biomolecules Laboratory, Faculty of Sciences, University of M'Hamed Bougara, Boumerdes, Algeria.

Corresponding author: so.toubal@univ-boumerdes.dz

Abstract:

Green synthesis of metal oxide nanoparticles from plant extracts is a promising alternative to the traditional physical or chemical synthesis method.

In recent years, the green synthesis of metal oxide nanoparticles has attracted considerable attention due to their very simple, efficient and eco-friendly protocol was developed to synthesize green nanoparticles using the extracts of various plants, due to their high capacity to produce a wide range of bioactive secondary metabolites with high reduction potential. notably polyphenols. This ecological method makes it possible to produce nanoparticles on a large scale compared to synthesis mediated by bacteria and/or fungi. These products are collectively called biogenic nanoparticles.

Iron oxide nanoparticles are widely used in the medical and pharmaceutical fields thanks to their diverse biological properties (antibacterial, antioxidant, insecticidal and anticancer).

Plant mediated synthesis of nanoparticles has been of great interest in the formulation of new pharmaceutical products.

Keywords : nanoparticles, biological properties, green chemistry, iron oxide.

Biocontrol potential of nettle botanical extracts against Culex pipiens, vector of vector-borne diseases

El Haddad Djillali[1], Toubal Souheyla[1], Kheddam Hocine[2], Merah Maroua[3], Boumaza Sarah[1],Benhabyles Narimen[1],

[1]*LBMAB, University M'Hammed Bougara of Boumerdes*

[2] *Department of Agronomy, UMBB University,Algeria.*

[3]*LBPBVP University of Saida, Algeria.*

Corresponding author: d.elhaddad@univ-boumerdes.dz

Abstract

Vector-borne diseases account for over 17% of infectious diseases and cause more than a million deaths each year. These are human diseases transmitted by vectors, such as *Culex* mosquitoes. However, the overuse of chemical insecticides has led to insect resistance. In order to limit the spread of these insects and contribute to sustainable environmental management, the insecticidal potential of botanical extracts from Nettle, namely aqueous and ethanolic extracts, was evaluated against fourth-stage larvae of *Culex pipiens* at concentrations ranging from 3% to 10%. Infrared analysis of *U. dioica* L. powder showed the presence of several molecules with various functions, including phenol (O-H), methylene (C-H), primary amines (N-H), nitro aromatic compounds (N-O), and aromatic ethers (C-O). The insecticidal activity of Nettle extracts showed very significant efficacy against L4 larvae of *C. pipiens* L. The mortality kinetics were directly proportional to the concentration used, as well as to the contact time of the larvae with the extracts. For the aqueous extract, better larvicidal activity was recorded with a CL50 value of 11.48 mg/ml compared to 12.74 mg/ml for the ethanolic extract. Furthermore, the ethanolic extract caused a faster mortality kinetics compared to the aqueous extract, with TL50 values of 6.25 hours and 19.92 hours respectively.

Nickel oxide nanoparticles: a review of their properties and applications in the medical field

Blizak Meriem Djanette [1], Bouchenak Ouahiba [1], Blizak Salah[2,3]

[1]*Bioinformatics, Applied Microbiology and Biomolecules Research Laboratory (BMAB), University M'Hamad Bougar of Boumerdes, Algeria*

[2]*Department of physics, Faculty of sciences, University Mohamed Boudiaf of M'Sila, Algeria*

[3]*Materials, Processes and Environment Research Unit (URMPE), University M'Hamad Bougar of Boumerdes, Algeria*

Abstract:

Nickel oxide (NiO) nanoparticles have sparked considerable interest because of their unique qualities and diverse potential uses. These tiny particles exhibit semiconductor properties and showcase stability in electrical, optical, and chemical aspects, along with catalytic characteristics. Notably, NiO nanoparticles have shown encouraging antimicrobial effects, indicating promise in combating various infections. Moreover, scientists are investigating their potential in cancer treatment, exploring their ability to target cancer cells effectively. Furthermore, NiO nanoparticles demonstrate antioxidant properties, which can help safeguard cells from oxidative harm. Their ability to absorb and emit radiation also makes them attractive for medical imaging purposes.

Given these outstanding attributes, NiO nanoparticles emerge as promising contenders for various applications, including infection treatment, cancer therapy, and medical imaging. Continued research endeavors aimed at unraveling their mechanisms and optimizing green synthesis methods, will facilitate the utilization of these remarkable nanomaterial in innovative applications, particularly in the medical field.

Approaches to Modeling Polymer Solution Viscosity: Insights from MLR, SVR, and ANN algorithms

Mohamed Kouider, Amar and Mohamed Hentabli
University Yahia Fares of Medea
Corresponding author: kouideramar.mohamed@univ-medea.dz

Abstact:
This study proposes a novel approach for predicting intrinsic viscosities of polymer solution mixtures using molecular descriptors for solvents and polymer monomers. The linear model (MLR), while offering some explanatory power, reveals notable discrepancies, prompting the exploration of alternative approaches. The Support Vector Regression-Radial Basis Function-Antlion Optimizer (SVR-RBF-ALO) demonstrates comparable accuracy to the simpler MLR model. However, the Artificial Neural Network-Antlion Optimizer (ANN-ALO) surpasses both models, exhibiting exceptional predictive performance. Optimized hyperparameters lead to a coefficient of determination (R2) of 0.7487 during testing, with the model's generalizability confirmed on the entire dataset (R2 = 0.7872). Notably, the low Mean Absolute Percentage Error (MAPE) values (13.3730% for the test set, 11.8329% for the entire dataset) highlight the accuracy and effectiveness of the ANN-ALO model in overcoming challenges associated with traditional linear and SVR models. The results of this study are logical with regard to the variation in experimental data, while highlighting the promising potential of the ANN-ALO algorithm in addressing the inherent variations in experimental data. This offers a robust and generalizable solution for predicting transformed intrinsic viscosity in polymer solutions.

Predicting Rheological Behavior: A Novel Approach Integrating ANN and ALO Algorithm for Starch Nano-Suspension Viscosity

Mohamed Kouider, Amar and Mohamed Hentabli
University Yahia Fares of Medea
Corresponding author: kouideramar.mohamed@univ-medea.dz

Abstact:
This study explores the rheology of suspensions containing solid particles in aqueous media thickened with starch nanoparticles (SNP). The objective is to model the viscosity of these mixtures across a diverse range of shear rates and varying amounts of SNP and SGHP (solid particles – SG hollow spheres). The modeling of suspension viscosity was conducted through the integration of artificial neural networks (ANN) and swarm intelligence algorithms. Utilizing a dataset of 1104 data points, the research emphasizes the significance of key features such as SNP proportions, solid particles of hollow spheres (SGHP) content, and log-transformed shear rate (LogSR) in predicting the log-transformed viscosity (LogViscosity). Three swarm algorithms-AntLion Optimizer (ALO), Particle Swarm Optimizer (PSO), and Dragonfly Algorithm (DA)—are evaluated for hyperparameter optimization in developing ANN models. The ALO algorithm emerges as the most effective, showcasing superior convergence, exploration, and exploitation capabilities. Regression analysis and comparative evaluations of ANN variants—ANN-ALO, ANN-PSO, and ANN-DA—reveal the robust predictive capabilities of ANN-ALO. Outperforming with an R2 of 0.9861, MAE of 0.1013, RMSE of 0.1356, and MAPE of 3.198%, ANN-ALO demonstrates consistent accuracy in predicting LogViscosity. While all models exhibit high alignment between predicted and actual viscosities, the ANN-PSO model has more limitations.

A New Approach for Phase Transition Confirmation using Equilibrium time of Total Energy; a computational Study

Chergui Yahia. Chergui, Essma. Salah. Redouane
IGEE, Boumerdes university
Corresponding author: y.chergui@univ-boumerdes.dz

Abstact:
We investigated Equilibrium Molecular Dynamics and Dl_Poly 4 to confirm the Phase Transition using the equilibrium time of total energy of Zinc Oxide Wurtzite Structure. Our system is composed from 2916 atoms (1458 atoms of Zn+2 and 1458 atoms of O-2) ; In this work we use isobaric and isothermal ensemble under the range of pressure 0-200GPa ad the rage of temperature 300-3000K, in order to study the behaviour of total energy versus pressure and temperature to extract the equilibrium time for confirming the phase transition comparing with available data. These results are only predictions which need an experiment confirmation

Ab-initio calculations of the structural and electronic properties of the t-Se1-xTex and for t-Se1-xTex containing a defect (t-Se1-xTex(D)) for low concentration (x = 0.03, 0.04 and 0.08)

Mekahlia Mahira

Laboratoire de Physique Appliquée et Théorique, L. P. A.T, Université Laarbi Tebessi Tébessa, Algérie

Corresponding author: mekahlia.maha.2014@gmail.com

Abstact:

In this research, we explore the structural and electronic properties of t-Se1-xTex and t-Se1-xTex containing a defect (t-Se1-xTex(D)) in the dihedral angle (ϕ) for low concentrations (x = 0.03, 0.04 and 0.08) utilizing WIEN2k code. Based on structural properties and highlighting the helical chain constants of t-Se1-xTex systems, it turns out that the distances of the two nearest neighbors (d1) and of the third neighbors (d3) increase, the valency angle (Θ) and the dihedral angle (ϕ) decrease when we substituted Se by Te, but, when x increases, d1 increases, d3, Θ and ϕ decrease compared to trigonal Se (t-Se). This is very identical to the experimental results. On the other hand, our defect did not significantly affect d1, whereas, d3 and Θ decrease, ϕ increases. The electronic properties show the semiconductor nature of both systems t-Se1-xTex and t-Se1-xTex(D), it also turns out that the gap decreases when increasing x in t-Se1-xTex compared to t-Se. likewise, the gap decreases when we introduce the defect in t-Se1-xTex, this is mostly due to the change in the p-orbital. Hence, intra-chain interactions have a role in determining the gap value for our systems; this is proven by the defect in ϕ. The control of the gap by changing x and by the defect opens real opportunities for applications like photovoltaic and optical storage.

Analyzing the Characteristics of Functional Half-Wave Plates in the Visible Spectrum

Z. Kebci, T. Zeghdoudi, A. Belkhir, O. Lamrous And F.I. Baida
Laboratoire de Physique et Chimie Quantique, Faculté des Sciences, Université Mouloud MAMMERI, BP 17 RP, 15000 Tizi-Ouzou, Alegria
Corresponding author: zahia.kebci@ummto.dz

Abstact:
The half-wave plate is an optical device capable of modifying the polarization state of the light transmitted through it. This study aims to optimise the parameters of a array of C-shaped apertures, engraved in a silver film, in order to design half-wave plates that are functional in the visible range. We simulate this structure using a numerical code based on the FDTD method. When an incident wave is linearly polarized at an angle $\theta=45°$ with respect to the x-axis, a phenomenon known as rotation of the polarization plane occurs. During the interaction of light with the half-wave plate, the component perpendicular to the plane of incidence undergoes a phase delay of π compared to the parallel component. Consequently, at the output of the half-wave plate, the two components are phase-shifted, resulting in a rotation of the polarization plane by an angle of $\varphi=2\theta$.

Quantum atomistic simulation and modeling of semiconductor nanomaterials for nanotechnology applications

Chaouki Siouani, Sofiane Safer, Sofiane Mahtout
University of Algiers 1, Algeria
Corresponding author: c.siouani@univ-alger.dz

Abstact:
A quantum atomistic simulation and modeling of pure arsenic Asn+1 and Ni-doped arsenic NiAsn (n =1-20) nano-materials used in various nanotechnology applications are reported in this work. Our computational investigation is based on the spin polarized DFT with the GGA approximation implemented in the SIESTA code.
Our theoretical investigation reveals that the transition metal atom Ni 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 NiAsn 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 Asn+1 and NiAsn 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 Ni atom in the cluster, the charge transfer and orbital hybridization.

In-Silico Study of a Metallic complex between N-Methyl Thiosemicarbazide Schiff Base and Co (II) against MCF-7 cell lines

Nour Hasni , Rayene Kadri, Mekki Kadri
LCP laboratory of physical Chemistry University of 8 Mai1954-Guelma
Corresponding author: nourhsn234@gmail.com

Abstract:
Thiosemicarbazone ligands are subgroup of hydrazine which have identical pharmaceutical abilities as their parent aldehyde/ketone groups. Further, the complexation of thiosemicarbazone ligand with transition metal, especially with Co(II), Ni (II), Cu(II), Zn(II) are widely studied because these are highly beneficial source of medicinal drugs due to their significant biological response to control the pathogen infection as a result of lipophilicity, chelation, hydrophobicity, structural diversification, good therapeutic index, penetration power etc. which are essential requirement for medicinal drug. So, the therapeutic applications of Co (II), Ni(II), Cu(II), Zn(II) complexes of thiosemicarbazone ligands are centre of investigation because of their significant properties as antioxidant , anticancer, anti-inflammatory , antimalarial, antimicrobial , anti-tuberculosis etc. Therefore, the thiosemicarbazone ligands based Co(II), Ni(II), Cu(II), Zn(II) complexes are celebrated class of coordination compounds for drug discovery. In this work, a molecular docking study was conducted aginst MCF7 cell line proteins (PDB ID : 1fdw, 2wtt, 5gwt). The compounds were tested against a human cancer cell line to study their cytotoxic potential as anticancer agents against breast cancer. Docking calculations revealed that the ligand and the corresponding complexes exhibited significant anticancer affinities.

Key word: N-Methyl Thiosemicarbazide, molecular docking, MCF7.

POSTER CONTRIBUTIONS

Valorization and development of a polyester polymer using Luffa fiber

Laib Nouri, Benyahia Azzedine, Deghfel Nadir
University of M'sila
Corresponding author: nouri.laib@univ-msila.dz

Abstract :
Natural fibers have been known for a long time and are used as reinforcement in the manufacture of composite materials. In particular, in the field of packaging, health, pharmacy, automobile manufacturing and in the aeronautical field. Natural fibers have many benefits such as; availability, low cost, low densities, rigidity, biodegradability and have significant mechanical behavior. Many researchers have observed that the preparation of natural fiber reinforced composite materials can improve the mechanical efficiency of these composites. Laib et al. prepared a composite material from an unsaturated polyester matrix with Luffa fibers, which underwent different chemical treatments (NaOH, permanganate, dichromate, silane and bleach) in order to improve the fiber-matrix iterfacial adhesion. The objective of this work is to study the effect of alkaline treatment and treatment time on the mechanical properties of a composite material based on a thermosetting matrix (unsaturated polyester) reinforced with Luffa fibers.

One-pot synthesis of copper nanoparticles

Asma Bahloul[1] , Samia Bouakkaz[1], Ali Benayahoum[2],
[1]*Laboratory of Applied Chemistry, University of 08 mai 45, Guelma, Algeria*
[2]*Scientific and Technical Research Center for Physical and Chemical Analysis (CRAPC), Algeria*
Corresponding author: basma2765@gmail.com

Abstract:

In the present work, we have elaborated copper nanoparticles with a chemical reduction of $CuSO_4$ copper ions, using N_2H_4 as principal reducing agent, and tea extract as stabilizing agent and secondary reducing agent under microwave irradiation. The DRX spectrum of the nanoparticles showed that the product is a Cu/Cu_2O alloy with a 40/60 ratio. The calculated average crystal size of Cu and Cu_2O is 29.734 nm and 32.02 nm respectively. The UV-Visible spectrum of the copper colloidal solution showed a characteristic peak of Cu_2O nanoparticles at 270 nm and a Cu peak at 578 nm. The BET analysis results show that the specific surface area of the synthesized nanoparticles is 23.209 m^2/g, the average pore radius is 7.23 nm and the total pore volume is 0.0839 cm3/g. SEM analysis shows that these copper nanoparticles have a uniform and homogeneous spherical morphology.

Keywords: nanoparticles, copper, microwave, Thea extract.

Structural and Optical Properties of $Ga2O3$ Thin Films

Messeddek Lobna , Louiza Arab, and Nouredine Sengouga
Université of Biskra
Corresponding author: lobna.messeddek@univ-biskra.dz

Abstract :
Gallium oxide has attracted attention as an alternative to other costly materials in their applications as solar-blind photodetectors. Several physical methods have synthesized it. This work synthesized gallium oxide thin films using a cost-effective spin-coating method on different substrates. Therefore, different substrates of samples are quartz, sapphire, and si. X-ray diffraction is performed to characterize the structure of the sample. The optical bandgap of $Ga2O3$ is calculated based on the transmittance value measured from UV-visible spectrophotometer, which ranges from 4.5eV to 5.1eV.

Green Nanomaterials for the Removal of Heavy Metals and Pollutants from Petroleum Wastewater Review

Khezzane Anouar, Saoud Abdesselam, Souhaila Meneceur
Faculty of Hydrocarbons and Chemistry, University of Boumerdes
Corresponding author: a.khezzane@univ-boumerdes.dz

Abstract:
For now it is a great research advancement which initiative the introduction of many green technologies for treatment of the water containing heavy metals (for instance, Cd, Pb, Zn) and organic pollutants (generally – organic substance). Obviously, being partial this time does drastically change the point of view. It becomes kind of a given thing that fully brings to life the persistence of those environmental issues. The very outer layer can give a lot of information about its contents. The oftentimes green nanomaterials, like ZnO@CuO and MgO@SnO2 are proved to be very strong heavy-metals and hydrocarbons sorbent compared to the other kinds nano-materials and they can efficiently remove over than 100% of these contaminants. This work shows that the green synthesis method is the right approach, and what this means is that when researchers will now be making ZnO,CuO and α-Fe2O3 nanocrystals to help the process of Pb(II), Bi(II) and As(III) pollutants which are released in oil wastewater. Summing up the discussion, one could say that there is no end in sight and nano-technology becomes the marker for benchmarking.

Effect of number of dips on Nanocrystalline titanium dioxide thin films prepared via dip coating

Hala Nezzal, Rahmane Saad, Elhachemi Guettaf, Temam Mohammed, Althamthami, Hachemi Ben Temam

Laboratory of Photonics Physics and Multifunctional Nanomaterials-University of Biskra

Corresponding author: hala.nezzal@univ-biskra.dz

Abstract:

Titanium dioxide (TiO2) is a widely employed material in various applications, including photovoltaic devices,diodes, gas sensors, optoelectronic devices, and photocatalysis, owing to its distinctive optical, electrical, and photocatalytic properties. In this research, we synthesized nanocrystalline thin films of TiO2 utilizing a cost-effective sol-gel dip coating method. We conducted an investigation into the impact of film thickness, which

was varied by altering the number of coating dips (ranging from 1 to 5 dips), on the material's properties. X-ray diffraction (XRD) analysis confirmed the presence of the anatase phase of TiO2 in all the samples, signifying the crystalline structure of the films. The optical characteristics of TiO2 were comprehensively assessed through UV-Vis spectroscopy, allowing us to gain insights into its absorption and transmission properties. This

evaluation sheds light on the films potential applications in the field of environmental remediation and water treatment, where their photocatalytic capabilities can be harnessed to mitigate the presence of organic pollutants.

Keywords: TiO2, Films, Thickness, Dip-coating, Photocatalysis.

Towards High-Performance Sodium-Ion Batteries: Synthesis and Comparative Caracterisation of BaAl2O4 and SrAl2O4 as Positive Electrodes.

Abdelali Benzaid, Nedjemeddine Bounar, Hadjer Merrouche, Doulfa Remmouche
University of Jijel
Corresponding author: abdelali.benzaid@univ-jijel.dz

Abstract:
In This work, we studied the Synthesis and characterization of spinel oxide compounds aluminate-based, by the solid method. The samples obtained BaAl2O4 and SrAl2O4 were characterized by two techniques: XRD and SEM. XRD results showed the presence of a spinel phase for both SrAl2O4 and BaAl2O4. They proved that the SrAl2O4 compound has a monoclinic structure with space group P1211 and lattice parameters a=5.1600Å, b=8.8220Å, and c=8.4440Å with a good refinement accuracy of 0.01 and that the compound BaAl2O4 has a hexagonal structure with space group P6322 and mesh parameters a=b=10.4490Å, and c=8.7930Å with a very good refinement accuracy of 0.001. The scaning electron microscopiy (SEM) images reveal that the BaAl2O4 sample is denser and contains fewer pores compared to the SrAl2O4 sample. this observation suggests that BaAl2O4could be a more promising choise as a cathode material for sodium-ion batteries.

Keywords: spinel oxides, synthesis, KRD, SEM, sodium ion battery.

Effects of Phosphorus Addition on the Structural, Mechanical, and the Magnetic Properties of FeCo Powders obtained by mechanical milling

Berkani Hanane
LPCM, Department of Physics, Faculty of Science and Technology, Eltarf University
Corresponding author: hananeberkani25@gmail.com

Abstract:
A high energy planetary ball-mill Retsch PM 400 was chosen for synthesis the nanostructured FeCoP powders at room temperature under an inert atmosphere for different milling times 0, 1, 2 and 3h. The characterization of the milled powders was carried out by XRD. The MAUD program which is based on Rietveld's method allows the overall profiles of the experimental diffraction patterns to be directly adjusted used as variables the instrumental characteristics in addition to the phase's formation, the structural, the microstructural and the mechanical parameters of the obtained powder mixtures. The magnetic properties are obtained VSM. The structural study revealed the coexistence of the centered cubic α-Fe(P) solid solution and Co75Fe25 binary phase, for all milled samples. The average crystallite size <L> of the formed solid solution and binary phase decreased with the milling time. The evolution of the mechanical properties "Young's Modulus and Poisson's Coefficient" demonstrated the stiffness and the deformation properties of the formed phase and solid solution. The milling process induced some important changes in the magnetic properties, whereas higher powders milling time (3h) exhibit higher, coercive field, Hc and the highest value of the saturation magnetization, Ms, is observed after one hour of the milling time.

Keywords : High energy ball milling, nanostructured FeCoP powders, XRD, Rietveld method, Mechanical properties, VSM, Magnetic properties.

Elaboration and electrochemical characterization of Ti–6Al–4V alloys

Hayette Boutarfa , Salih Hamdi , Samah Adjmi .
Chadli Bendjedid University, 36000 El Tarf, Algeria.
Corresponding author: boutarfa-hayette@univ-eltarf.dz

Abstract:
Titanium and its alloys have attractive characteristics (good corrosion resistance, high mechanical characteristics, low density, transformation by conventional processes, etc…). They are used in the chemical engineering, the automobile, the marine applications aerospace, military, and biomedical industries, especially Ti-6Al-4V alloy. In this work, we carried out an experimental study of the electrochemical mechanism of cerium oxide on a Ti-6Al-4V substrate. (Titanium 90%, Aluminum 6% and Vanadium 4%, Titanium grade 5), was prepared by electrodeposition from dissolution of cerium nitrate Ce(NO3)3.6H2O in a mixed ethanol solution (50% water and 50% ethanol) at a concentration of 0.01 mol.l-1. The deposits were produced at room temperature at 21 degrees , during different electrodeposition times (900s, 1800s and 3600s) by imposing different current densities: -0.5, -1 and -2 mA/cm². We used X-ray diffraction analysis (XRD) to characterize the engineered coatings.
Keywords: Electrochemical characterization, Ti-6Al-4V and X-ray diffraction analysis (XRD).

Effects of substrate and Al doping on gallium oxide thin films

Amraoui Fatma, Sengouga Noureddine, Lobna Messeddek.
Affiliation of the participant: Laboratory of metallic and semiconducting materials LMSM, Mohamed Khider University, Biskra
Corresponding author: fatma.amraoui@univ-biskra.dz

Abstract:
Gallium oxide is a promising material for optoelectronic devices development. It is emerging in the field of wide-bandgap semiconductors for various applications. In this study, the structural properties of undoped and aluminum-doped gallium oxide (Ga2O3) thin films deposited on quartz and sapphire substrates by sol-gel (spin coating) are analyzed using XRD. To the best of our knowledge, no experimental report on Al-doped gallium oxide thin films is available at this time. the optical properties of doped gallium oxide by the sol-gel method are analyzed. Therefore, the annealing temperature of the samples is set at 1050 °C. The optical bandgap of films is calculated based on the transmittance value measured from a UV-visible spectrophotometer, which ranges from 4.8 eV to 5.0 eV. Scanning electron microscopy of the prepared samples revealed dense surface morphologies.

Overcoming Asphaltene Precipitation in Oil Production: A Look at Nanotechnology and Nanoinhibitors Review

Bendas Sarra , Hamada Boudjema

Affiliation of the participant: Faculty of hydrocarbons/university of boumerdes

Corresponding author: s.bendas@univ-boumerdes.dz

Abstract:

asphaltene precipitation and deposition which is a main hurdle to oil production, the rate of oil flow decreases due to this situation by pipe clogging. Thus, this concern is the figure out if the producers can be guaranteed to take preventive measures like assessing the stability of their products or using available and already used strategies (ex. lowered flow rates or chemical inhibitors). However, the main focus is on a promising new approach: Nanotechnology is a particular branch of science that crossed the border of bringing-up the production and exploitation of the nanoparticles, which of them are within 1- 100 millionth meters in size. The fields of nano technology and the chemistry incorporated with nanoscience have been keeping abreast with the speed of changing studies by using magnesium oxide (MgO) and nickel oxide (NiO) nanoparticles as "nanoinhibitors" which help to reduce asphaltene deposition age. These nano-inhibitors are able to pick up and capture asphaltene molecules that help bind in asphalt molecules within the oil that will keep it together. It is the effectiveness of these nanoparticles that resides on the types of nanoparticles used, surface area of nanoparticles as well as the specific environment where from the recovery takes place. The technology which is based on nanoparticle selecting and which is water-washable gives great results and involves a high interest from the part of people in disadvantaged conditions.

Isolation and characterization of cellulose nanofiber (CNF) from Algerian Lygeum Spartum using chemo-mechanical Method

Sabrina Ahmima, Nacira Naar

Affiliation of the participant: Macromolecular Synthesis and Thio-Organic Macromolecular Laboratory, Faculty of Chemistry, USTHB.

Corresponding author: sabrina.ahmima@gmail.com

Abstract:

Nowadays, the attention has shifted to environmentally friendly materials and bioproducts. Cellulose, the most abundant polymer, provides a sustainable source of nanocellulose. Also, nanosized cellulose has sparked widespread interest due to its numerous applications, including cosmetics, medicinal, fillers, and nanocomposite, due to its versatile properties such as biodegradability, stiffness, high surface area, higher mechanical properties, thermal properties, porosity, and flexibility. The latest advancements in green synthesis and technology encourage the maximum use of green methods of nanocellulose extraction. The aim of the study was the extraction of CNF from Lygeum spartum (Sparte) by a chemo-mechanical method. First, the fibers were subjected to different chemical treatments to eliminate non-cellulosic compounds, The chemically treated fibers were mechanically separated into nanofibers using ultrasound and homogenization. The obtained CNF was characterized by FTIR, XRD, TGA, and SEM. The FTIR results show the removal of hemicellulose and lignin, while XRD confirms the presence of cellulose I, the thermal analysis reveals that the thermal stability increases for the isolated nanofibers. The outcome of the study implies the possibility of nanofiber extraction from a new source using green methodologies, these nanofibers present a prominent alternative of synthetic fibers in large applications, especially in manufacturing green composites.

Synthesis, characterization, and Anticancer potential of ZnO nanoparticles

Hanane Mouada and Ilham Ben Amor
Affiliation of the participant: CU Tipaza
Corresponding author: mouada-hanane@univ-eloued.dz

Abstract:
In recent years, the utilization of biogenic materials for the synthesis of nanoparticles has gained significant attention due to its eco-friendly approach and potential biomedical applications. In this study, we explore the biosynthesis, characterization, and anticancer potential of zinc oxide (ZnO) nanoparticles using shrimp shells as a novel and sustainable source. The biosynthesis of ZnO nanoparticles was achieved through a simple, cost-effective, and environmentally friendly method, harnessing the natural bioreductive properties of shrimp shells. The synthesized nanoparticles were thoroughly characterized using various analytical techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Fourier-transform infrared spectroscopy (FTIR). Subsequently, we assessed the anticancer potential of these nanoparticles against various cancer cell lines, shedding light on their promising role in cancer therapy. This study highlights the sustainable and biocompatible synthesis of ZnO nanoparticles from shrimp shells and underscores their potential as a valuable asset in the fight against cancer. Additionally, we employed molecular docking studies to gain insights into the interactions between the ZnO nanoparticles and specific cancer-related molecular targets.

Parametric XRD Rietveld Refinements of FeBP Alloy Milling

Sabah Baara, Fatma Baara, Hanane Berkani,Locif Redouani and Wassila tebib

Affiliation of the participant: Laboratory of Physicochemistry of Materials (LPCM), Sciences and Technology Faculty,University of Chadli Bendjedid, El Tarf, Algeria

Corresponding author: baarasabah36@gmail.com

Abstract:

The mechanical alloying process has been successful in preparing a wide range of alloys using various methods, showcasing significant advancements in ball milling techniques. The main goal is to remove the fraction of atoms located in defective environments such as grain boundaries (GB), which tend to detach from surfaces, as well as their junctions, pores, and lattice defects. The solid-state reaction between pure elements during ball milling occurs gradually through repeated fracturing and cold welding, accompanied by pronounced deformation of crystal lattices. This study seeks to investigate the correlation between phase composition and the impact of milling on the solid-state reaction in Fe-B-P alloys. The focus is on examining the interdependence of these factors and their influence on the formation of solid solutions and the behavior of stored energy in the milled powders.

Keywords: Mechanical alloying, Fe-B-P, Powder, solid solutions.

Synthesis and Characterization of pure ZnO, pure CuO, and 50% ZnO/50% CuO nanocomposite

Boughanem Mohd Oulmessaoud, Touka nassim, Tabli dalila
Affiliation of the participant: *University of Akli mohand oulhadj Bouira*
Corresponding author: m.boughanem@univ-bouira.dz

Abstract:
In this work, pure ZnO, pure CuO, and 50% ZnO/50% CuO nanocomposite were effectively prepared and deposited on a glass substrate by the sol gel spin coating method. Various characterization techniques, such as X-ray diffraction analysis (XRD) and UV-Vis spectroscopy, were used to investigate the crystal structure and optical properties. The XRD results showed that the crystal structure of CuO is monoclinic, and that of ZnO is hexagonal. The particle sizes of 12.88nm, 18.06nm, and 11.73nm were measured for pure CuO, pure ZnO, and 50% ZnO/50% CuO nanocomposite. The results of UV-Vis spectroscopy indicate that the band edge absorption is red-shifted.

Effect of the annealing temperature on the band gap of TiO_2 nanaotubes

Zalouk Djedjiga, M.S. Belkaid, D.Hatem, D.Hocine, S.Boudinar, A. Kadri, T. Hadjersi

Affiliation of the participant: UMMTO

Corresponding author: djedjiga.zalouk@ummto.dz

Abstract:

The present work reports on the effect of thermal annealing on physical properties of high aspect ratio self-organized TiO2 nanotube layers formed by anodization of Ti foil. The obtained TiO2 nanotubes were annealed at different temperatures between 300°C and 900°C for 3 h. The morphological caracterization schow that The tubular form of TiO2 begins to gradually evolve from the temperature of 700°C and approaches that of nanoparticles until the latter become predominant above 800°C with is related to the phase transition anatase to rutile or directly Ti- rutile the results schow that From the whole range of temperatures (300-900 °C), annealing at 600 oC leads to the formation of crystalline TiO2 nanotube layers with mixed anatase-rutile structure offering the best optical properties with a law reflexion (7%) corresponding to the lowest value of the optical band gap of 2.59eV. This properties allows the use of TiO2 nanotube as photoanode in solar cells and photocatalysis.

Key Words: nanotubes, mixed phase, band gap, temperature, nanoparticles.

Development of biomaterials based on biopolymers for drug encapsulation with biomedical applications

Mohammed Dellali , Kheira Zanoune , Camelia Elena Iurciuc (TINCU) and Marcel Popa

Affiliation of the participant: Faculty of Technology , Hassiba Benbouali University of Chlef

Corresponding author: m.dellali@univ-chlef.dz

Abstract:

The objectives of our study was to obtain oxidized carboxymethylcellulose (CMCOx) by oxidation of CMC in the presence of sodium periodate in order to create a new functional group, respectively the aldehyde function (-CH=O) capable of to react with the amine groups (-NH2) of chitosan (CS) by forming covalent bridges of the Schiff base type (-C=N) between the chains of two polymers. The existence of aldehyde groups in CMCOx was demonstrated by FT-IR and NMR spectroscopy. Hydrogel films were prepared based on CS and CMCOx by crosslinking using different molar ratios between the aldehyde groups of CMCOx and the amine groups of CS. The conversion index of amine groups into Schiff bases from the hydrogel films obtained and the swelling capacity were determined. Several influencing parameters have been brought into play and have been studied, such as the molar ratio , the time and the temperature of crosslinking. The selected films were characterized by the analyzes of FTIR, SEM, TGA, mechanical resistance. Curcumin was encapsulated in the films obtained based on CS/CMCOx. The release kinetics of curcumin from the films obtained and the permeability of the skin membrane were evaluated in vitro in two different pH solutions (pH=5.5 and pH=7.4) using a diffusion cell Franz. Hydrogel films can be optimized to obtain delivery systems with dermatological applications.

Keywords: Skin cancer ; Hydrogel film ; polysaccharide ; Encapsulation, release system.

New systems based biopolymer- superparamagnetic nanoparticles - anticancer molecule for cancer therapy

Kheira Zanoune, Mohammed Dellali, Corina-Lenuța Savin, Marcel Popa

Affiliation of the participant: Faculty of Technology , Hassiba Benbouali University of Chlef, Algeria,

Corresponding author: k.zanoune@univ-chlef.dz

Abstract:

Cancer is one of the deadliest diseases in the world. Controlled drug delivery systems offers great opportunities for the development of new non-invasive strategies for the treatment of cancers and the main advantage of these systems is represented by their capacity to accumulate in tumors by enhanced perme ability and retention effect. We focused our research on hybrid magnetic nanoparticles (nanospheres) based on chitosan obtained by double crosslinking in reverse emulsion. Hybrid nanoparticle consisting of a polymeric matrix in which is dispersed a magnetic nanoparticles material (magnetite (Fe3O4), maghemite (γ-Fe2O3), hematite (α-Fe2O3), etc.), are lately studied for use as target delivery systems of antitumor drugs. Selection of the matrix-forming polymer is based on the need for it to be biocompatible, biodegradable, mucoadhesive, possessing reactive functional groups in order to achieve the cross-linking process under mild reaction conditions. The hybrid nanoparticles nanospheres formed is characterized in order to determine their shape and size; these particles are from a few tens to a few hundred nanometers in diameter. SEM confirmed their nanometric size and their well-defined spherical shape. These nanospheres allowed the encapsulation of an increased amount of 5-Fluorouracil and presented a controlled drug release.

Keywords : Chitosan, nanospheres, Biomaterial, hybrid nanoparticles, magnetite, 5-Fluorouracil.

Elactroplating of nickel and manganèse alloys on Copper

Hizia Merkoune, Kamel Hachama, Chafiaa Ait Ramdane

Affiliation of the participant: Khemis Miliana university
Corresponding author: hizia.merkoune@univ-dbkm.dz

Abstract:
Many nanomaterials have several applications, the electroplating of some materials is an electrochemical technique that can improve the quality of final products of this operation Zinc, nickel, manganese, cobalt and others have a catalytic property wish give them a big importance, we try to give some electrochemical characteristics of manganese and nickel alloys on copperl. Electrochemical behavior of electroplating of those alloys is studied by cyclic voltammetry with defferent compositions of the bath are experimented to see how is their effect on the deposition of those materials.

Antifungal activity of nanoparticles cobalt ferrite with doped lanthanum

Debboub Salima[1], Barhouchi Badra [2], Chidouh Amina [3], Tahraoui Tarek [4]

[1]*Laboratory of Materials Elaboration and Analysis, Badji Mokhtar-Annaba University, Annaba, Algeria. Department of Physics, Chadli Bendjedid University, El Tarf, Algeria*

[2] *Pharmaceutical Sciences Research Center (CRSP), Constantine, Algeria*

[3] *Department of natural sciences, Higher Normal School of Technological Education of Skikda, Algeria*

[4] *L3M Laboratory, National Higher School of Technology and Engineering - ENSTI Annaba, Algeria*

Corresponding author: debboub-salima@univ-eltarf.dz

Abstract:

The co-precipitation method is used to synthesize nanoparticles of lanthanum (La)-doped cobalt ferrite (CoLa0.1Fe1.9O4NPs). The nanoparticles are chiefly characterized by X ray scattering analysis (XRD) to find out their mean size as well as the distinct phases. The antifungal activity of CoLa0.1Fe1.9O4NPs is mainly assessed against a clinical yeast, C. albicans. The NPs has shown amazing antifungal activity. Nanoparticles have foremost applications in the biomedical field.

Synthesis and characterization of a new supported CuO semiconductor

Ouardia Zekri, Thiziri Djelloudi
Affiliation of the participant: USTHB
Corresponding author: ouardiazekri@yahoo.fr

Abstract:
In the last few decades, the semiconductors have been extensively used to mineralize toxic and nonbiodegradable environmental pollutants by heterogeneous photocatalysis. However, most of them have some disadvantages, such as low quantum efficiency, low specific surface area, and low adsorption capacity, which significantly limit the efficiency of photocatalysis. The immobilization of a semiconductor on a suitable matrix can exhibit a higher photodecomposition of organic and inorganic pollutants than the bulk oxide. In fact, the immobilization of semiconductors on various supports promote catalytic reactions by offering more active sites, also permit the recycling, and reuse of the catalysts. In this work, we report the synthesis and characterization of a new immobilized CuO semiconductor on a hexagonal mesoporous silica (1.25%Cu/HMS). This nanomaterial was characterized by X-ray diffraction, N2 adsorption-desorption, ultraviolet and visible diffuse reflectance spectroscopy.

Key words: semiconductor, CuO, immobilization, nanomaterial.

Environmental and Health Risks: Adsorption of Methylene Blue by Phosphate/Zeolite Composites

Djalila Boudemagh, Tahani Achouak Chinar, Mona Bendouda, Derradji Chebli, Ehab Alshamaileh

Affiliation of the participant: Ferhat Abbas University, Setif1,

Corresponding author: djalila.boudemagh@gmail.com

Abstract:

The environmental and health impact of synthetic dyes used in various industrial processes is considerable. Some of these dyes is released into liquid effluents without prior treatment, which posing a risk to human health and the environment due to their stability and low biodegradability. Among them, methylene blue, a harmful pollutant, poses serious health risks. Inhalation or ingestion may cause eye burns, difficulty breathing, nausea, vomiting and other unpleasant symptoms.To moderate these risks, several research studies on the use of phosphates and zeolites compounds have been carried out due to their specific physicochemical properties. The objective of this work is therefore to evaluate the adsorption capacity of phosphate/zeolite composites on methylene blue dye. The prepared samples were characterized by Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD).

Key Words: Zeolite, calcium phosphate, IR, depollution, Bleu of methylene

Elaboration and characterization of CuAlTe2 by self propagating high temperature synthesis (SHS)

Saad-Hamideche Linda[1], Tobbi Ouafa[2], Benzerouk Hayette[3], Chouit Fairouz[3]

[1] *Departement of Physics,Faculty of Ssciences Exactes ,University of Frères Mentouri, Constantine 1,Constantine 25000, Algeria.*

[2] *Department of sciences and technology, Faculty of technology, University Batna 2, Constantine Avenue, Fesdis, Batna 05078, Algeria.*

[3] *Departement of technology, Faculty of Technology, 20 Aout 1955, University,P.O 26, Road El-Hadaik, Skikda, 21000, Algeria.*

Corresponding author: saadhamideche.linda@umc.edu.dz

Abstract:

CuAlTe2 films were produced using a novel technique known as auto combustion or self-propagating high-temperature synthesis (SHS) via thermal evaporation. This process involved depositing the films on a cold-pressed mixture of Cu, Al, and Te powder. The as-grown films had a chalcopyrite structure with a preferred orientation along the (112) direction, with lattice constants of a=6.058 Å and c=11.98 Å. SEM analysis revealed that the resulting thin films had a nanostructured morphology. Furthermore, a direct band-gap of 2.08 eV was observed.

Keywords: CuAlTe2, auto combustion, DRX, SEM analysis,optical properties, band gap.

Zinc Oxide nanoparticles elaboration via chemical means: Sol-Gel, and green synthesis for photocatalytic activity

Bessaad Asma, Toubal Bedreddine, Toubane Mahdia
Affiliation of the participant: Algiers university
Corresponding author: a.bessaad@univ-alger.dz

Abstract:
In this work, two different methods were adopted for the synthesis of ZnO NPs: Sol-Gel and green synthesis, with citrus extract serving as an essential component. Firstly, Zinc Acetate [Zn(CH3CO2)2.2H2O] ,CAZ = 0.2 M, was dissolved in distilled water at room temperature for 30 minutes (sol 1). Then Sodium Hydroxide NaOH, CNa OH = 2 M, was also dissolved in distilled water at room temperature for 30 minutes (sol 2). Subsequently, using a pipette, sol 2 was added dropwise to the first solution under agitation at room temperature for 2 hours until reaching the desired pH. The solutions obtained were left for a necessary period for the powder to precipitate, and sometimes a centrifuge is used for the speed of precipitation. Afterwards, the obtained powder was rinsed five times with distilled water. However, for the preparation of ZnO NPs using citrus extract, the aqueous salt solution was prepared by dissolving 0.2 g of zinc (II) acetate dihydrate [Zn(CH3CO2)2.2H2O] in 50 mL of distilled water with stirring for 15 minutes. Then, 20 mL of citrus extract was added at room temperature, and the desired pH was achieved with a sodium hydroxide (NaOH) solution. Finally, the solution was sonicated for 30 minutes at room temperature, followed by centrifugation at 6000 rpm at 15 °C for 10 minutes and placed in the incubator to dry at 80°C.

Keywords: ZnO nanoparticles, Sol-Gel, Green synthesis, Citrus extract.

Synthesis, characterization and evaluation of antioxidant activity for metal oxide nanoparticles

Latra Benkhira, Ferhat Mohammed Fouad, Messai Ridha, Bounedjar Nourelhouda, Ben Aissa Abir.

Affiliation of the participant: El oued University

Corresponding author: latrabenkhira1@gmail.com

Abstract:

Applications of metal oxide materials, have proven to be very successful in the fields of medicine, cosmetics, and food preservation. Since they have special physical and chemical properties, they have also been used as filters for efficient wastewater treatment. The antioxidant activity will be studied in this work using copper-doped zinc oxide nanoparticles. Fourier transform infrared (FT-IR), ultraviolet-visible (UV-Vis), X-ray diffraction and scanning electron microscopy were used to analyze the produced nanoparticles.

Synthesis and characterization study of graphene oxide (GO) and Zinc oxide decorated reduced graphene oxide (ZnO-rGO) nanocomposite

Berrehail Marwa, Aicha Bensouici, Naima Touafek, Noudjoud Hamdouni & Ouahiba Halimi

Affiliation of the participant: University of Constantine 1

Corresponding author: marwa.berrehail@doc.umc.edu.dz

Abstract:

In this study, we are interested by synthesis and FTIR characterization of GO and ZnO-rGO nanocomposites. Two steps synthesis was used to obtain the samples: GO was synthetized using Modified Hummers method with a different mass ratios (1:2; 1:3 and 1:4, graphite: potassium permanganate) during the first step. ZnO-rGO samples were obtained after refluxation at 100°C during 120 min. FTIR characterization technique was carried out to study chemical bonds vibrations of our nanocomposites. FTIR spectra show the peaks located at 1039.89 〖cm〗^(-1) and 2920.04 〖cm〗^(-1) peaks in all ZnO-rGO sampels, corresponding to the C-O and C-H bonds. This result exhibits that the graphite is not well oxide. The peaks presents in ZnO-rGO spectrum are 3252.27 cm-1 and 1043 cm-1 for the vibration of the O-H and C-O, and the new weak inensity peak located at 830.32 cm-1 is attributed to the Zn-O bond.

Development and characterization of a flexible silicone/zno-fe piezoelectric sensor

Rabehi Saliha, Saidi.M, Ouabadi.N, Hammouche.H, Achour.H, Chaouchi.A, Laghrouche.M, Rguiti.M, Christian.C, Ben Achour.M
Affiliation of the participant: UMMTO
Corresponding author: saliha.rabehi@ummto.dz

Abstract:
Our study focuses on the production of a flexible piezoelectric sensor based on silicone/ZnO-Fe composites by hot compression for an energy recovery application. We began our work by synthesizing iron-doped zinc oxide nanopowder using the sol-gel method, followed by the production of flexible composite films. Dielectric and electrical characterizations were carried out.

Kinetic and microstructural analyses of enstatite formation from nano-oxides

Laziri Khadidja, Foudil Sahnoune, Amar Djemli
Affiliation of the participant: Physics and Chemistry of Materials Lab, Faculty of Science, University Mohamed Boudiaf of M'sila
Corresponding author: khadidja.laziri@univ-msila.dz

Abstract:
In this work, we prepared a forsterite-enstatite composite using the solid-state reaction method, using nano-oxides through the sintering process. Advanced techniques like (DTA, SEM, and EDS complementary techniques were used. Our thermal analysis showed at a lower heating rate of 2°C/min; the estatite phase formation was detected as the first peak and forsterite phase formation as the second peak using DTA analysis. Model-free methods were used to determine the activation energy of enstatite crystallization, such as Kissinger-Akahira-Sunose (KSA), Flynn–Wall–Ozawa (FWO), Kissinger, Ozawa, and Boswell methods. The activation energy of enstatite is constant while decreasing as a function of crystallization fraction. Based on the experimental data, the S˜esta´k Berggren (SB) model was found to be suitable in describing the kinetic model; the kinetic parameters (n, m) and ln(A) were 1.06, 0.53, and 48.60, respectively. The enstatite mechanism reaction was controlled by nucleation followed by linear nuclei growth. The SEM/ EDS analyses of the forsterite-enstatite sample confirmed the reaction mechanism, where a secondary enstatite phase with rod shape grains length of 0.68 µm. EDS analysis detected an elemental composition matching the theoretical composition of enstatite.

Microstructural, and dielectric properties of rare-earth (RE) zirconates whith Pyrochlore structure

khawla djilat, Amar Djemli, Djaida Redaoui, Foudil Sahnoune, Nouari Sahebd

Affiliation of the participant: materials physics and applications laboratory.Higher Normal School of Bou-Saada

Corresponding author: djilat.khawla@ens-bousaada.dz

Abstract:

Pyrochlores are regarded as the most prominent compounds among high-entropy oxides for future practical applications, owing to their varied properties, such as thermal conductivity, and excellent high-temperature stability. Pyrochlore ceramics can be fabricated by different methods, the most often utilized techniques are solid-state reactions, combustion synthesis, and the sol-gel method.

In our work we have synthesized medium-entropy pyrochlore oxide RE2Zr2O7with solid state reaction method. The dielectric properties, crystal structure and microstructure of our compound have been investigated, such as the value of the activation energy . AC conductivity, dielectric constant, dielectric loss, impedance spectroscopy, and electrical modulus of our compound sintered at 1550 ◦C, and the Coefficient of thermal expansion determined by using the dilatometer. In order to characterize the phase compositions of the medium-entropy pyrochlore oxide at various temperatures, the X-ray diffraction (XRD) was exploited. Using a field-emission scanning electron microscope equipped with energy-dispersive spectroscopy (EDS), the microstructures and elemental distributions were determined.

Effect of Cr addition on the microstructural and Structure properties of nanostructured (Fe0.7Co0.3)100-xCrx alloys

Dhehbi Housseyn, A. Guittoum, M. Hemmous, D. Martínez-Blanco, J.A. Blanco, P. Gorria

Affiliation of the participant: university Blida 1

Corresponding author: dehbi.housseyn@gmail.com

Abstract:

In this work, we have studied the effect of Cr addition on the microstructural and hyperfine properties of the nanocrystalline ternary (Fe0.7Co0.3)100-xCrx (X = 0, 5, 10, 15 and 20 at. %) powders were elaborated by high energy ball alloying for a milling time of 72 h using X-ray diffraction (XRD) and SEM photographs. The SEM photographs show the variation in the in-particle size, shape and morphology, when the Cr content increases. Quantitative EDX analysis confirms the absence of the contaminants and the starting stoichiometry conservation. When the Cr content increases from 0 to 15 at.%, . X-ray diffraction patterns show the formation of a disordered bcc-Fe(Co,Cr) solid solution. The lattice parameter, a (Å) and the lattice microstrain ε (%) increase up to a critical Cr content (Xcrit= 10 at.%), beyond the critical content, these parameters decrease progressively with increasing Cr content. The average grain size, D (nm), decreases to 65 % of its initial value (x= 0 at.%) after an addition of Cr to the elaborated compositions.

Synthetization and Characterization of a series of Nanomaterials Lamellar Double Hydroxides (LDHs)

Haffaf Wissem, M. Hamouni and Z. Abdelsadak.

Affiliation of the participant: University Abubekr Belkaid, Faculty of Science, Macromolecules Research Laboratory (MRL),Tlemcen, Algeria.

Corresponding author: wissemhaffafdz@gmail.com

Abstract:

In the present work, a series of Lamellar double hydroxides (LDHs) materials were synthesized by using aluminium (Al3+) as a trivalent cation (M3+) with varying M2+ divalent cations such as magnesium (Mg2+), zinc (Zn2+), and calcium (Ca2+) ions to prepare magnesium–aluminium-layered double hydroxide (MgAl-LDH), zinc–aluminium-layered double hydroxide (ZnAl-LDH), and calcium–aluminium-layered double hydroxide (CaAl-LDH), respectively. The samples were prepared by the co-precipitation method with a molair ratio M2+/M3+=3. The structure, the morphology and the thermal stability of the different phases prepared were investigated using X-ray diffraction (XRD), Fourier transform infrared spectra (FT-IR), thermogravimetric analysis and differential thermogravimetric analysis (TGA/DTG). The powder XRD patterns revealed that only the MgAl-LDH and ZnAl-LDH phases exhibited the typical layered double hydroxide structures, while the CaAl-LDH had different phases. Additionally, the TGA curves showed a two-step degradation behavior for the samples.

In conclusion, the synthesis method used in this work, was effective only for the preparation of magnesium-aluminum-layered double magnesium–aluminium-layered double hydroxide (MgAl-LDH) and zinc–aluminium-layered double hydroxide (ZnAl-LDH).

Ti3C2 MXene : synthesis, characterization and applications on biosensing

Zermane Maroua, Teniou Ahlem, Rhouati Amina, Berkani Mohammed.

Affiliation of the participant: higher national school of biotechnology

Corresponding author: maroua.zn@gmail.com

Abstract:

This study presents a comprehensive investigation of MXene, a two-dimensional material, including its synthesis, characterisation and innovative application in biosensing. MXenes, derived from layered MAX phases, exhibit unique properties such as high conductivity, large surface area and biocompatibility, making them promising candidates for biosensing platforms.

The synthesis methodology involves selective etching of the aluminium from MAX phases to obtain MXene nanosheets. FTIR analysis reveals the presence of functional groups and provides insight into its surface chemistry, while XRD analysis confirms the crystal structure and phase purity. SEM imaging further confirms the morphology and microstructure of MXene, which is essential for understanding its properties. The unique properties of MXene make it an ideal candidate for biosensing applications. This research explores the integration of MXene into FRET-based biosensors for antibiotic detection, offering advantages such as enhanced signal amplification, improved detection limits and real-time monitoring of biomolecular interactions. In this study, a MXene-based FRET biosensor was developed to enable accurate and rapid detection of amoxicillin in complex samples. The high conductivity and large surface area of MXene facilitate efficient energy transfer between donor and acceptor molecules, resulting in improved sensitivity and selectivity of the biosensor.

Preparation and characterization of a composite for dye adsorption: Modeling of nonlinear isotherm and kinetics

Sardi Amina, Kradra Brahma Khadidja, Bennabi Souad
Affiliation of the participant: Département de Chimie, Faculté Science Exacte Et Informatique, Université Hassiba Ben Bouali, , Ouled Fares, 02010 Chlef, Algeria.
Corresponding author: a.sardi@univ-chlef.dz

Abstract:
Dyes and pathogenic microorganisms are among the major pollutants in the environment, resulting from the massive increase in the global population and industrial activities. They are not only hazardous to human health but also harmful to our ecosystem, leading researchers to test and evaluate other effective, low-cost, and environmentally friendly materials in order to minimize these impacts. Among these important and popular materials, natural bentonite clay stands out, having been widely and primarily explored as a support material for the preparation of nanocomposites. This is due to its abundance, low cost, environmental compatibility, and key characteristics such as high cation exchange capacity, swelling layers, and significant specific surface area. Our work focuses on preparing polymer-based nanocomposite materials supported on bentonite using various methods. The prepared nanocomposite materials are then characterized using different analytical methods such as X-ray diffraction (XRD), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), and Fourier-transform infrared spectroscopy (FTIR). The nanocomposites will be evaluated for catalytic reduction of organic pollutants as well as antibacterial agents against pathogenic bacteria.

The effect of the size of the hardening precipitates formation after T5 heat- treatment on the microhardness of the Al–Si based alloys

Sersour Zakia[1] and Amirouche Lynda[2]
[1]*Laboratoire Revêtement, Matériaux et Environnement, UMBB, Algeria*
[2]*USTHB, Algeria*
Corresponding author: z.sersour@univ-boumerdes.dz

Abstract:
The presence of magnesium and copper in the A356 and AS10G alloys results in the formation of the hardening precipitates such as Mg2Si and Al2Cu. The effect of Mg and Cu, on the formation of this phases in both as cast and heat treated Al-Si alloys containing 0.22–0.44-wt% Mg and 0.01–0.1-wt% Cu has been investigated. A qualitative microstructural examination and Vickers microhardness , were carried out to study the effect of T5 heat treatment consisting of direct aging at 500°C for aging times ranging from 0.5 h to 8h on the formation the hardening precipitates in the alloys A356 and AS10G.
Plotting isochronal microhardness versus aging temperature curves, has uncovered a peculiar behavior: all the investigated aging times are marked by a hardness minimum that is reached at 400°C. The observed drastic drop in hardness has been interpreted in terms of Mg2Si and Al2Cu clusters dissolution that have formed due to natural aging. The melting point of such nanoscale particles is supposed to be lower than that of the typical hardening precipitates due to size effects. As a result, a thermal treatment, at T=400°C, is suggested to get rid of any kind of nanoscale clusters forming during natural aging.

Keywords: hardening precipitates size, microstructure, micro-hardness.

Photocatalytic activity of green synthetized ZnO nanoparticles for antibiotics and synthetic dyes

Laila Hamza , S. Laouini, H. Ali Mohammed, S. Menaceur
USTHB University, Algeria
Corresponding author: laila.hamza.2009@gmail.com

Abstract:
This study aims to addresses the environmental pollution caused by antibiotics and synthetic dyes in aquatic eco-system, presenting a novel method for their degradation. Zinc oxide (ZnO) nanoscale photocatalyst were synthesized through green synthesis method using an extract derived from lemon peels. The synthesized materials were extensively characterized through UV spectrophotometry, X-ray diffraction (XRD), scanning electron microscopy (SEM), The results showed different morphlogies of ZnO NPs, with average sizes of 20 nm. The ZnO NPs exhibited optical bandgap energies of 3.2 eV. Under natural sunlight irradiation, The ZnO NPs demonstrated exceptional photocatalytic activity, achieving a remarkable degradation rate 98.8 %, for metronidazole and 90 % for ciprofloxacin in just 12 min. Additionally, ZnO nanoparticles removed 84 % of toluidine blue and 77 % of Congo.

Elaboration and characterisation of CuAlTe2 by Thermal evaporation

L. Saad-Hamideche, O. Tobbi, H. Benzerouk, F. Chouit.
Departement of Physics,Faculty of Ssciences Exactes ,University of Frères Mentouri, Constantine 1,Constantine 25000, Algeria.
Corresponding author: saadhamideche.linda@umc.edu.dz

Absract:
CuAlTe2 films have been deposited by Thermal evaporation onto a mixture of Cu, Al, and Te powder that was cold-pressed. The as-grown films exhibited a chalcopyrite structure with a preferred orientation along the (112) direction, and their lattice constants were determined to be: a=6.058 Å and c=11.98 Å. SEM analysis revealed that the resulting thin films had a nano-structured morphology. Additionally, a direct band-gap value of 2.08 eV was observed.

Keys words: CuAlTe2, thin films, structural properties, optical properties, band gap.

Study of the annealing effect in the crystallization of hydrogenated amorphous silicon induced by Nickel

Ouafa Ben Azouz, Faouzi Kezzoula, Mohamed Kechouane
USTHB University, Algeria
Corresponding author: wafbenaz@gmail.com

Abstract:
In this work, we emphasis on the Nickel (Ni) induced crystallization (NIC) of hydrogenated amorphous silicon (a-Si: H) thin films. Hydrogenated amorphous silicon (a-Si:H) films were deposited by DC cathodic sputtering on glass (corning) with a forming gas (Ar+H) flow of 10 sccm. Hydrogenated amorphous silicon have been crystallized by using thin Ni layer deposit on it. Thin layers of nickel deposited on the (a-Si: H) films using DC by physical vapor deposition system. Ni and (a-Si:H) were deposited on substrate(corning) by DC sputtering in the same deposition chamber within 10 min base pressure: 5. 10-3 mbar. The samples (Ni/a-Si :H/ substrat) have then annealed at different temperatures (400°C, 500 °C and 550 °C) in isochrones stages during 6 hours. The (NIC) of hydrogenated amorphous silicon based on annealing process, annealing experiments performed under N2 atmosphere. The effect of annealing temperature on Nickel induced crystallization of hydrogenated amorphous silicon has been evaluated using X-ray diffraction, and Raman spectroscopy, in order to check the crystallinity of obtained samples after annealing. The influence of the Ni layer thickness on the crystallization of hydrogenated amorphous silicon (a-Si: H) has also studied. In this study, the structure properties of the Poly-Si films crystallized by annealing of Ni-induced have been investigated.

Elaboration and Characterization of chitosan nanoparticles

Benouared Noussaiba and Laribi Hassiba
Saad Dahleb Blida University
Corresponding author: nou.benouared95@gmail.com

Abstract:
Chitosan, a natural polysaccharide, is extensively used in medical formulations. It is derived from chitin and is found as the primary component of cell walls of fungi, the exoskeletons of crustaceans and insects, and scales of fish. Chitosan is a cationic polymer composed of (1–4)-2-amino-2-deoxy-β-ᴅ-glucan. Due to its pH sensitivity, biocompatibility, and bioactive functions, chitosan is widely used because of its non-toxic, biodegradable, and biocompatible properties. This research aims to study the formation of chitosan nanoparticles and to characterize these nanoparticles based on their morphology and cross-linking with TPP (tripolyphosphate). Chitosan nanoparticles were produced using the ionic gelation method. Briefly, 0.5% chitosan was dissolved in 1% (v/v) acetic acid and filtered through a 0.45 µm filter membrane. The filtered solution had its pH adjusted to 5 using NaOH. Then, a 0.2 mg/mL TPP solution was added dropwise into the aqueous system under stirring at 800 rpm for 1 hour. The suspension was centrifuged, and the precipitate was air-dried and collected as a fine powder for further analysis. The morphological form was characterized SEM, while morphological exploration was conducted FTIR spectroscopy. The size of the nanoparticles was found to be on a nanometer scale. The formation of these nanoparticles can be observed through FTIR analysis, which shows the functional bond between chitosan and TPP. The FTIR spectrum indicated that cross-linking was successfully carried out, while the SEM study proved that the chitosan nanoparticles were well-dispersed spherical shapes with good particle size distributions.

Study the growth of indium oxide (In2O3) thin film using ultrasonic spray

Bourhefir Ranida, Saidi Hanane, Hamani Nedjette, Attaf Abdellah, Ben khetta Okba, Djehiche Nour el Houda
Université Mohamed Kheider, Biskra
Corresponding author: ranida.bourhefir@univ-biskra.dz

Abstract:
Indium oxide (In2O3) is a material belonging to the group of transparent conductive oxides, which are widely used in many fields of technology including optoelectronics and photovoltaics. However, the properties of In2O3 thin films depend on many factors. Therefore, the aim of the study was a thorough investigation of the properties of In2O3 thin films of various thicknesses. Indium oxide thin films were deposited by ultrasonic spray at different deposition times to investigate the influence of deposition time on the optical and electrical properties of thin films. The optical properties and electrical characteristics of these layers were investigated by UV-Vis-NIR spectrophotometer and four-point probe. It is observed that the optical transmittance spectra with high transmittance of more than 80 % for all samples at the visible and near-infrared ranges. Furthermore, the electrical properties of this film change with deposition time increase.

Comparative Study of Thin-Film Nickel Oxide and Zinc Oxide Nanostructures for Renewable Energy Applications

H. Benzerouk[1], M. Mekhnache[1], F. Chouit[1], A. Boussaha[1], L. Saad HAmideche[2],

[1]*Department of Technology, Faculty of Technology, 20 Aout 1955 University Skikda, 21000, Algeria*

[2]*Departement of Physiques, Faculty of Exact Science, Mentoury University, Constantine, 25000, Algeria*

Corresponding author: h.benzerouk@univ-skikda.dz

Abstract:

This study aims to compare thin-film layers of nickel oxide and zinc oxide prepared using spray pyrolysis for their performance in renewable energy applications. The performance of the prepared nanostructured layers was evaluated through a series of experimental tests, including photovoltaic conversion efficiency, performance stability under different conditions, and environmental stress resistance. We prepared two different solutions with a molarity of 0.2 mol/L each, starting from zinc acetate dissolved in ethanol to obtain zinc oxide layers and nickel chloride dissolved in distilled water to obtain nickel oxide layers. These layers were deposited on glass substrates and heated to 400°C. For a comprehensive understanding of the crystalline and optical properties, we employed a range of methods, including XRD, SEM, and spectrophotometry, and compared the obtained results with those of other studies. The results demonstrate that both materials are considered good candidates for use in renewable energy and have a nano-scale crystalline length. Zinc oxide is considered an n-type semiconductor, while nickel oxide is a p-type semiconductor.

Keywords: ZnO, Thin-film deposition, NiO, Nanostructured materials, Photovoltaic conversion.

Properties of nanocystalline Ni-P coatings

A. Boussaha, S. Alleg, J. J. Suñol
University 20 Aout 1955- Skikda
Corresponding author: asma.boussaha20@gmail.com

Abstract:
In this study, the nanostructured Ni-P coatings are obtained by electrodeposition on a copper substrate using a watt's bath ((NiSO4, 6H2O: 0,2M / NaH2PO2 , H2O : 0,1M and H3BO3 : 0.005 M) with the additive. The saccharine addition to the bath was effective in the lowering the grain size of the deposits. Electrodeposition experiments were performed at 70°C. The Ni-P coatings are obtained at three different potential, -1,3 V-1,15Vand -1 V. The time of the deposition was 20 mn. The evolution of microstructure and mechanical properties of Ni-P coatings was studied by X-ray diffraction and micro hardness measurements. The Rietved refinement of the XRD pattem reveals the formation of an amorphous phase and Ni (P) solid solution with two structures Ni(P)-1 and Ni(P)-2. The non-homogeneity of the Ni(P) solid solution is evidenced by the existence of two bcc structures having the differents lattice parameter, crystallite size and proportions. The crystallite (~10 nm). However, the crystallite size of the Ni(P)-2 phase increased from 51 nm to 89 nm by increasing the potential from -1,3V to -1V. The amorphous fraction reaches a maximum value of about 26 %. The values of the microhardness is 665.4 Hv0.3. The microhardness values of the deposits increased with decreasing the crystallite size of Ni(P)-2 phase. Codeposition of P in the Ni matrix apparently causes a significant increase in microhardness compared to pure nickel electrodeposits (about 220 Hv).

Keywords: Nanocrystallin, deposits, Electrodeposition, XRD.

Structural Characterization of Lanthanum Orthoferrite ($LaFeO_3$) Synthesized via Solid-State Route

Belguenoune Ahmed, Ouldhamadouche Nadir, Bassaid Salah, Dehbi abdelkader, Chakour Naziha
Université Ibn Khaldoune Tiaret
Corresponding author: ahmed.belguenoune@univ-tiaret.dz

Abstract:
LaFeO3 exhibits interesting semiconductor behavior because of its distinct electronic structure and bandgap properties. As a semiconductor with a wide bandgap (around 2.0-2.5 eV), it shows great potential in applications like photovoltaics, photocatalysis, gas sensors, and solid oxide fuel cells due to its chemical stability and catalytic activity. This study offers valuable insights into the structural characteristics of LaFeO3 perovskite prepared using a solid-state reaction technique. The nano-crystalline LaFeO3 orthoferrite material was effectively produced via solid-state reaction at a calcination temperature of 850°C, employing Fe2O3 and La2O3 as initial reagents. Comprehensive examinations involving X-ray diffraction, Rietveld refinement, and Fourier transform infrared spectroscopy validated the orthorhombic space group Pbnm, with an average particle size of 48 nm for the resulting powder after annealing at 1100°C. The analyses also precisely determine the atomic positions and lattice parameters while confirming the presence of FeO6 octahedral in LaFeO3. This comprehensive characterization not only enhances our understanding of LaFeO3 but also facilitates its tailored optimization for specific semiconductor applications. Keyword: Perovskite, LaFeO3, Rietveld, FTIR, DRX.

Elaboration and characterization of mixed phosphate

Ounnoughi Hadjer [1], Boudemagh Djalila [1], Chebli Derradji [2]
[1] *Advanced Ceramics Laboratory, Emerging Materials Research Unit, Ferhat ABBAS Sétif 1 University.*
[2] *Chemical Process Engineering Laboratory, Department of Process Engineering, Ferhat ABBAS Sétif 1 University.*
Corresponding author: hadjerounoun@gmail.com

Abstract:
Phosphate chemistry was developed rapidly during the last forty years of the twentieth Century. The diversity of applications of phosphate-based compounds The Human Body Contains about 1% by weight of this element, more than 85% of which is present in bones and Teeth in the form of calcium phosphates. It is also the basis of some products Pharmaceutical products and can be used in animal feed, in the manufacture of Detergents, food preservation and as fertilizers for land fertilization ; In this study, barium-based mixed phosphates were developed and Characterized by IR, SEM and XRD analyses.

Elaboration of fluorine doped ZnO Thin Films grown on the glass Substrate previously heated at 350°C by SP Process and their Physical and optical properties

Salah Boulmelh, L. Saciand Azizi Assia
LEMEAMED laboratory, Departement of Electronics, Universityof frères Mentouri, Constantine 1, Algeria.

Abstract:
This work deals with an experiment study of some physical properties of undoped and doped thin films (ZnO:F). The films were deposited by fully automated spray pyrolysis deposition technique (SP) on the microscope glass substrate previously heated at 350°C. The starting solution is a mixture of an equivalent mass of 0.1 mol of [Zn $(CH_3COO)_2$, $2H_2O$] and previously specified quantity of (NH4F), the latter is dissolved in a mixture of deionized water and ethanol with a ratio of 4:2 respectively. The XRD spectra of all samples shows the appearance of different diffraction peaks correspond to ZnO phase. The calculated values of lattice constants were found around a=b=3.24 Å and c=5.20 Å. The average particle size of the samples was found between 9 and 67 nm. The Raman spectroscopy showed the presence of the E_2^{low}, E_2^{high}phonon modes attributed to wurtzite phase of ZnO. On the other hand, the optical study enabled us to measure the transmittance, the latter was used to extract band gap and Urbach energy. Sprayed (ZnO:F) films transmit 40 - 90 % of the visible light. The evidence of this study is that the band gap is slightly affected by the proportion of fluorine (3.25 eV - 3.28 eV) and is inversely proportional to the Urach energy (101 meV – 147 meV). This study showed that the deposited films can be used as windows layer in solar cells devices.

Key words: Zinc oxide; Spray pyrolysis; Zinc acetate-dihydrate; Raman spectroscopy.

Effect of HF on the grain size, the electrons mobility and photocatalysis activity of TiO2 thin films

Fayçal Bensouici[1], Abd Alaziz Abboudi[1], Sabrina Iaiche[1], Abdelkader Djelloul[1], Mohamed Bououdina[2], Muhammad Humayun[2]

[1]Laboratory of Structures, Properties and Interatomic Interactions, Faculty of Sciences and Technology, Abbes Laghrour University, Khenchela Algeria
[2]Department of Mathematics and Sciences, College of Humanities and Sciences, Energy, Water, and Environment Lab, Prince Sultan University, Riyadh 11586, Saudi Arabia
Corresponding author: bens_faycal@univ-khenchela.dz

Abstract:
In this work, we have successfully fabricated bare TiO2 and fluorine (F) doped TiO2 thin films via the sol-gel dip-coating technique on the soda lime glass substrates. The effect of fluoric acid (HF) concentration on the structural, optical, photocurrent and photocatalytic properties of TiO2 thin films is investigated. The films are characterized by XRD technique, SEM, EDS, AFM, and UV-visible spectrophotometer. The XRD patterns show the presence of highly crystalline anatase phase TiO2 and the decrease of grain size whith increasing the molar ratio of HF. The SEM images reveal some cracked surfaces, while the EDX reveal the absence of fluorine in all samples. The AFM images exhibit a decrease in roughness with the increase in HF concentration. UV-visible spectrometry reveals high transparency in the visible region (about 85%) and the shift in absorption edge toward the higher energy side. The photocatalytic activities and the electron mobilities test shows a decrease in the degradation rate of MB and the electron mobilities with the decease of grain size. This work will trigger the development of highly efficient acid-modified photocatalysts for environmental remediation.

Keywords: Fluorine, titanium oxide, organic dye, thin films, photocatalysis.

Synthesis of ZnO -Co3O4 nanocomposites by hydrothermal method

Azizi Assia [1], S. Harrat[1], A. Naceri[1], Nadjah Sobti[1] and L. Saci [2]

[1] *Phases Transformation laboratory, Departement of Physics, frères Mentouri University of Constantine 1, Algeria.*

[2] *LEMEAMED laboratory, Departement of Electronics, frères Mentouri University of, Constantine 1, Algeria.*

Corresponding author: azizi_ssia@yahoo.fr

Abstract

The main objective of this work is to develop ZnO-based nanocomposites. A series of nanocomposites was prepared by hydrothermal method. The different obtained nanostructures were systematically characterized in terms of structure and morphology using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Raman spectroscopy. The XRD diffractograms of all samples showed the crystallization of the hexagonal wurtzite structure of ZnO phase with nanoscale crystallites, and the clear appearance of the second phase Co3O4 when increasing the concentration of cobalt acetate, which was confirmed by SEM images. Energy-dispersive X-ray spectroscopy (EDS) spectra confirmed the formation of ZnO/Co3O4 nanocomposite without any impurities. The vibrational analysis by Raman spectroscopy confirmed the good crystallization of the wurtzite structure, as evidenced by the presence of the E2 (low) mode observed at 99 cm-1, and showed that the ZnO lattice was disrupted due to the increase in cobalt acetate concentration. The antibacterial test was conducted using the Kirby-Bauer agar diffusion method. The efficacy of these nanocomposites in the antibacterial test is negative when the concentration of cobalt acetate exceeds 30%.

Key words: ZnO, nanostructures, green synthesis, poppy leaf extract, AFM, Photocurrent.

Structural, morphological, optical characterization and photocatalytic activity of $BiMnO_3$ thin filmprepared by sol gel.

O. Allouane[1], M. Toubane[2], M.Tazerout[3], K. Ayouz[4] , N. Beldjoudi[1]

[1]*Faculté de physique U.S.T.H.B; Algérie*

[2]*Research Unit on Materials, Processes and environment University M'hamedBougara of Boumerdes*

[3]*Research Center in Technologies-CRTI, P.O. Box 64, Cheraga, 16014 Algiers, Algeria*

[4] *Research Center in Technologies-CRTSE. Algeria*

Abstract:

Bismuth manganese ($BiMnO_3$) thin film was deposited by Sol- Gel dip coating technique on glass substrates to investigate the structural, morphological and optical properties for photocatalyticapplication.The film annealing at 500° for 2h is characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), UV visible spectrophotometer and photocatalytic test degradation of methylene blue solution in order to obtain the correlation between physical and chemical properties. Resultindicated the formation of single crystalline phase $BiMnO_3$ indexed in a monoclinic structure. The morphological characterization show smooth and continuous films. Finally, to calculate the gap energy E_g of these layers we have reported the optical properties such as absorption and transmittance response. The optical results report a large band absorption in the UV- visible and small band gap.

Keyswords: $BiMnO_3$, gap energy, Sol-Gel technique.

Elaboration and characterization of doped ZnO thin films

S. Bouhouche[1], A. Otmani[2], M. Toubane[1] and F. Bensouici[3]
[1] *URMPE Unite,UMBB University, 35000 Boumerdes, Algeria*
[2] *LRPCSI, 20 Aout 1955 University, 21000 Skikda, Algeria*
LASPI2A, Faculty of Sciences and Technology, Abbes Laghrour University, Khenchela 40.000, Algeria
Corresponding author: sabouhou@yahoo.fr

Abstract:
In this research work, structure, microstructure, optical, electrical and photocatalytic properties of undoped, and Erbium doped ZnO thin films prepared by sol-gel dip-coating are investigated. The precursor solution of undopedZnO was prepared using zinc acetate dihydrate, ethanol and mono-ethanolamine as staring material, solvent and stabilizer, respectively. In the solution, Zn2+ concentration was chosen as 0.4 M.Doped ZnO solutions were prepared by adding erbium nitrate pentahydrate (Er(NO3).5H2O) X-ray diffraction (XRD) results showed that all deposited films crystallize under the hexagonal wurtzite structure, with a preferential orientation along the (002) plane. SEM results show that undopedZnO films consist of uniform, spherical grains forming dense, homogeneous films.Transmission spectra show that the average transmittance of all Er-doped films is around 75%. Photocatalytic activity of the films evaluated by methylene blue photodegradation shows that undopedZnO films exhibit higher photocatalytic activity than Er-doped ZnO films, reaching 95% after 5h under UV irradiation.

Keywords: ZnO thin films, sol-gel, Er doped ZnO, DRX, phtocataly

Elaboration and characterization of biodegradable Biocomposite based on polysaccharides and plasticized with DL-lactic acid.

Djalila Aoufi , Fayrouz Benhaoua, Nabila Belloul
Research Center In Industrial Technologies -CRTI- EChahid Mohammed ABASSI Cheraga, Algiers; Algeria.
Corresponding author: aoufidjalila@yahoo.com

Abstract :
The aim of the present work is the development and characterization of new formulation of biodegradable composite based on starch/cellulose blend and DL-lactic acid as new plasticizer. The cellulose used in this study is a mixture of particles of micro and nano order. Our study consists in evaluating of the influence of the DL-lactic acid content on the behavior of obtained films. The physicochemical characteristics of the obtained coating were highlighted by different techniques (FT-IR, sorption isotherm, TGA, and water vapour permeability). The developed films are studied in order to use them as new formulations to produce food packaging. The obtained films are generally homogeneous, thin, and slightly flexible. All films were easily removed from the glass plate and show visually smooth surfaces. DL-lactic acid (LA) was chosen as a plasticizer. Its presence in the films brought about a chemical modification of the polymer which was highlighted by the Fourier transform infrared analysis. The hydration properties, the solubility coefficient and the water vapor permeability have been improved.

Improvement of the sintering temperature of a lead-free ceramic material of the type $(Ba_{0.85}Ca_{0.15})(Zr_{0.1}Ti_{0.9})O_3$ by the addition of a copper oxide CuO.

Rabah Amrani[1], Malika Saidi, Ahcène Chaouchi[1], Nouara Lamrani[1], Yannick Lorgouilloux[2], Mohamed Aymen Ben Achour[2], Mohamed Rguiti[2], Christian Courtois [2]

[1]*LCAGC, Faculty of Science, UMMTO*

[2] *University. Polytechnic Hauts-de-France, INSA Hauts-de-France, CERAMATHS- Materials and Processes Department, France.*

Corresponding author: rabah.amrani@ummto.dz

Abstract :

The most widely used piezoelectric materials are lead-based, in particular the PZT $(PbZr_{1-x}Ti_x)O_3$ family, which is used in many applications as pulse generators, ultrasonic transducers, sensors, actuators, positioning devices or piezoelectric motors. However, the presence of lead in these materials is harmful to human health and the environment. Consequently, a number of studies are focusing on the development of lead-free materials capable of replacing PZT, such as BCZT$(Ba_{0.85}Ca_{0.15})(Zr_{0.1}Ti_{0.9})O_3$. Since the synthesis and production of the material (BCZT) is generally carried out at high sintering temperatures in excess of 1400°C. In our study, we used additives (sintering agents) such as CuO to lower the sintering temperature. Various characterization techniques were used to characterize pellets, including XRD and SEM. The XRD pattern of the synthesized powder indicated that the composition crystallizes in a perovskite structure without any secondary phase at a temperature of 1300°C/2hour. A study of the dielectric and piezoelectric properties of ceramics sintered at1300°C/2hour showed that they exhibit out standing properties: high dielectric permittivity (εr) and low dielectric losses (tanδ).

Keywords: Dielectric, piezoelectric, BCZT, sintering agents, CuO.

Electrochemical metal deposition on silicon nanowires

A. Larbi-Didouche[1], S. Lamrani[1], M. Toubane[2], S. Fadel[1], A. Manseri [3], R. Belhoucif[1], S. Abaidia [1].

[1]*Laboratoire Revêtement, Matériaux et Environnement, UMBB, Boumerdes, Algeria*

[2]*URMPE Unit, M'hammedbougaraUniversity, 35000 Boumerdes, Algeria*

[3]*Research Center of Semi-conductor Technology for Energy, CRTSE-02, Bd Frantz FANON,Algiers.*

Corresponding author: aichadidouche19@gmail.com

Abstract

Silicon based nanostructures, like silicon nanowires (SiNWs)have a wide range of possible applications(like optics, photocattalytic, renewable energyand biological sensors)whether they are combined or not with other materials by means of various methods.

In this work, we reportaMorphologicalstudy of Silicon Nanowires (SiNWs) elaborated using Ag assisted electroless chemical etching at room temperature. Prior the etching, Ag nanoparticles (AgNPs) were deposited in a HF/$AgNO_3$ solution. The Si samples coated with AgNPs were immersed, for 60 min, in H_2O_2/HF solution to perform a chemical etching.The chronoamperometry method was used to obtain ametallic nanoparticlesdeposited on SiNWs substrate.The morphological study, performed using a Scanning Electron Microscopy (SEM), shows perpendicular nanowires having diameters in the nanometer range and a length of 15µm. And a non- uniform deposition of metal on the ends of nanowires.

Keywords: Silicon nanowires, Metal-assisted chemical etching, SEM.

Synthesis and physicochemical characterization of ceo_2-x%lif nanocomposite

Chikhaoui Imane[1], Lamrani Nouara[1], Guhel Yannick[2], Kennour Sadia[1], Oughanem M'hand[1], Saidi Malika[1], Douani Rachida[1] Chaouchi Ahcène[1], Amrani Rabah[1], Boudart Bertrand[2].

[1] *Laboratory of Applied Chemistry and Chemical Engineering, UMMTO, Algeria*

[2] *Normandie Université, UNICAEN, ENSICAEN, CNRS, GREYC UMR 6072 14000 Caen, France*

Corresponding author: imane.chikhaoui@fs.ummto.dz

Abstract :

In this study, the sol-gel method was used to prepare pure CeO_2 nanoparticles. Simultaneously, to enhance the material's properties as a humidity sensor, composites were produced by incorporating lithium fluoride (LiF) in varying proportions (X%) into the CeO_2 nanoparticles. The structural, and electrical characteristics of the pure CeO_2 nanoparticles and composites were investigated using characterization techniques such as X-ray diffraction,and scanning electron microscopy. Sensitive layers based on these nanoparticles were deposited on specific electronic structures to form humidity sensors. The results of the electrical characterizations demonstrated that the incorporation of 10% LiF significantly improves the humidity detection properties of the CeO_2 nanoparticles. These materials exhibit enhanced properties as humidity sensors, thus opening new prospects for their application in efficient and sensitive humidity detection devices.

Keywords: CeO_2, fluorine structure, composite, lithium fluorid, sol-gel, humidity sensor, impedance spectroscopy.

Study of the influence of powder granulometry on paste rheology

Isma Bozetine, Fatima Boudeffar, Ali mameri, Amar Manseri, Abdelhak Cheriet, Aissa Keffous.

Centre de Recherche en Technologie des Semiconducteurs pour l'Energétique, 2, Bd Frantz Fanon. BP 140, Alger 7M, Alger

Corresponding author: bozetineisma@yahoo.fr

Abstract :

The aim of this work is to study the influence of powder granulometry on paste rheology and on the quality of the deposits made with these powders. Our work therefore consists in manufacturing silicon pastes for electrodes used as anodes in lithium batteries. Silicon paste consists of silicon powder as the active material, carbon powder as the conductive agent and PVDF as the binder. We prepared two pastes with two different Si grain sizes, namely PSi1 and PSi2, with Si grain sizes of 283 and 111 nm respectively. The characterization methods used were scanning electron microscopy MEB and laser granulometry. The results of the characterizations showed that the granulometry and morphology of the powders influence the quality of the deposits as well as their adhesion to the substrates.

Keywords: Silicon, granulometry, MEB, characterization.

Enhancing Solid Oxide Fuel Cells: A Study on the Impacts of Operating Temperature on Nano-Materials Properties

Sarah Guenou, Ali Cheknane, Imane Benseggane
University of Laghouat
Corresponding author: s.guenou@lagh-univ.dz

Abstract :
SOFCs have gained attraction as viable options for clean and effective energy conversion due to their low emis-sions, high energy efficiency, and fuel flexibility. However, operational temperature has a significant impact on SOC performance and durability. For the purpose of comprehending the behavior of the cell and maximizing its per-formance, the temperature dependency of electrode reactions including oxygen reduction and fuel oxidation is essential. Additionally, tempera-ture influences the electrolyte and electrode materials' conductivity and dif-fusivity, which in turn impacts the total cell impedance and polarization. Additionally, the impact of temperature on the nano-materials used in fuel cells such as yttria-stabilized zirconia for the electrolyte, nickel-based cermet for the electrode, and alloys that form chromia for the inter-connect is investigated. Designing robust and effective SOFC systems re-quires an understanding of the thermochemical and mechanical properties of these nano-materials under working conditions. The present review un-derscores the complex correlation between temperature and solid oxide fuel cell (SOFC) performance. In order to further improve the performance and economic viability of SOFC technology, future re-search directions are also explored. They include developing temperature-dependent modeling, characterization methods, and materials development.

Structural and morphology properties of NiP nanocoatings

Kacel Tawous, Mebarki Mourad, Hemmous Messaoud, Djama Mustapha
Research Center in Industrial Technologies (CRTI), Algeria
Corresponding author: t.kacel82@gmail.com

Abstract:
In this work, Ni-P nanocoatings with different surface morphologies were electrodeposited from Watts bath using direct (DC), current techniques. The effect of cycle numbers on the evolution of microstructure, structural properties such as the lattice parameters and the mean grain sizes of composites were investigated. We found that the I200/I111 ratios are small relative to those of NiP powder, indicating a strong <200> texture for all sample, the variation of the lattice parameter, a (Å), with cycle numbers indicates that the films are subjected to a compressive stress and we observed the relaxation when cycle numbers increasing. The mean grain sizes D are between 47 and 78 nm. The variation of D with the cycle numbers shows a maximum equal to 78 Å corresponds to a cycle numbers equal to 2. The morphology properties of coatings are studied by scanning electron microscopy (SEM) technique.

Keywords: NiP, nanocoatings, DRX, SEM, electrodeposition.

Synthesis Mechanisms, Characterization, and Optical Bandgap of Metal halide perovskites nanoparticles: ABI3 (A: K; B: Cu)

Meriem Filah[1], Hana Terbah[2], Dalila Mouattah[2]
[1] *Laboratory of materials for applications and valorization of renewable energies (LMAVER), University of Amar Telidji , BP37G 03000 Laghouat, Algeria*
[2] *Laboratory Physico- Chemistry of Materials (LPCM), University of Amar Telidji , BP37G 03000 Laghouat, Algeria.*
Corresponding author: m.filah@lagh-univ.dz

Abstract
This work aims to investigate the synthesis methods of Metal halide hybrid perovskites materials as nanoparticles with controlled sizes, compositions, and morphologies. In addition, their characterizations with X-ray diffraction (XRD) and UV.V were also carried out to confirm the purity, the crystallinity, the particle sizes, and the bandgap values. In this experimental work, a special hydrothermal synthesis route of ABI3 (metal halide perovskites with A: alkali metal, B: transition metal) nanoparticles under various conditions is presented as well as a discussion about the phases, the particle size evolution, and the values of band-gap.The results revealed the crystallization of different metal halide perovskites phases (with A: K; and B: Cu). Furthermore, the nano-particle sizes were also confirmed and calculated using the Scherrer formula. On the other hand, the optical band gap values verified with Tauc Plot estimation of all previous nanopowders, exhibited their optical proprieties, which confirms that these metal halide perovskites are exceptional candidates for photovoltaic applications.

Keywords: Metal halide perovskites, X-ray powder diffraction, Bandgap.

Study of the microstructural characteristics of Al-Si based alloys and correlation with their mechanical properties

Sersour Zakia[1], Boughideh Yacine[2] and Boukherroub Nadia[3]
[1]*Laboratoire Revêtement, Matériaux et Environnement, UMBB, Algeria*
[2] *Department of physics, University of Boumerdes, Algeria*
[3]*UR-MPE, M'hamed Bougara University, Boumerdes, 35000, Algeria*
Corresponding author: z.sersour@univ-boumerdes.dz

Abstract:
In the current study, the effects of additives and T6 heat-treatment temperature on the microstructural and hardness properties of Al-Si eutectic and hypo-eutectic alloys, destined to automotive industry are investigated. The investigated alloys are divided into two different groups: Al-11.9wt%Si (B413), Al-11.67wt%Si-0.22 and Al-7.2wt%Si-0.44wt% Mg (A356). These groups of alloys have been investigated after T6-tempers, with aging at 160°C for 4h, after solutionizing at 540°C for 8h, followed by quenching in cold water and after T7 tempers with aging at 230°C for 4h, after the same processes of solutionizing and quenching. Different characterization techniques have been used for microstructural examination namely: optical microscopy, scanning electron microscopy, Energy Dispersive Spectrometry, as well as X-Ray Diffraction. The hardness properties have been measured by using Brinell-durometer. Our alloys' microstructure revealed that the different nanoscale intermetallic phases, such as the α-$Al_{15}(MnFe)_3Si_2$, β-Al5-Fe-Si, π- $Al_8FeMg_3Si_6$ and Al_7Cu_2Fe iron-rich compounds, as well as the Al_2Cu and Mg_2Si hardening precipitates, have been formed during solidification and after T6-tempers.

Keywords: Microstructural examination, nanoscale intermetallic phases, hardening precipitates size, Brinell- hardness measurements.

Magnetism in AlNiCo

Drifa Brinis
M'hamed Bougara University, Boumerdes, 35000, Algeria
Corresponding author: brinisd@yahoo.fr

Abstract:
The AlNiCo family belongs to the family of hard ferromagnetic materials. They are desired for their thermal stability (stable magnetization at high temperature) and they are used as permanent magnets due to their square hysteresis curve. Nevertheless, one of the drawbacks of the alloy is its low coercivity which can be improved by adding the Iron (Fe). Also, the adding of Cooper (Cu) and titanium (Ti) can increase the the saturation magnetization of the alloy. In our work, we aim to study the influence of Fe, Cu and Ti at different percentages, on the magnetic performance of the alloy.

Keywords: AlNiCo, ferromagnetic, hysteresis curve

Green Synthesis and Characterization of Light-Responsive ZnO Nanostructures

Narimene Bouza, Nadjah Sobti, Azizi Assia and L. Saci
LEMEAMED laboratory, Departement of Electronics, frères Mentouri Universityof, Constantine 1, Algeria.
Corresponding author: Narimene.bouza@doc.umc.edu.dz

Abstract:
This research explores the green synthesis of nanostructures using plant extracts, an emerging field in nanotechnology. The present study focuses on the synthesis of zinc oxide (ZnO) nanostructures via a spray pyrolysis method utilizing poppy leaf extract. Poppy leaf extract was employed to synthesize ZnO nanostructures deposited on copper substrates using spray pyrolysis method. The synthesized ZnO nanostructures were subsequently characterized using various techniques, including X-ray diffraction (XRD)**,** atomic force microscopy (AFM) analysisand electrochemical measurements. XRDanalysis revealed that theZnO nanostructures exhibited well-defined crystallographic orientations. The AFM image analysis revealed that the ZnOnanostructures had a very smooth and dense surface morphology with a low surface roughness value of 344.3nm.The results of the current-voltage (J-V) measurements indicate a higher current density for the ZnO nanostructures under light illumination, suggesting photocatalytic activity. Additionally, the electrochemical impedance spectroscopy (EIS) results suggest an improvement in the catalytic performance of the ZnO nanostructures.

Keywords: ZnO, nanostructures, green synthesis, poppy leaf extract, AFM, Photocurrent.

Fabrication of a dual-response intelligent/ active bio-films and its application in shrimp preservation

Sadi Amina, Ferfera harrar hafida, Benhalima Tayeb
Chimie macromoleculaire USTHB
Corresponding author: sadi.amiiina@gmail.com

Abstract:
Green functional food packaging films based on crosslinked carboxymethyl cellulose/gelatin (CMC/Ge) as the matrix were developed by incorporating Ge-montmorillonite nanoclay (OM) as a nanofiller, anthocyanins (ATH) extracted from red cabbage as a colorimetric indicator, and pistacia leaf extract (PE) at varying concentrations as an active agent. These films, produced through a casting method, underwent comprehensive characterization using FTIR spectroscopy, XRD, UV-vis spectroscopy, SEM, AFM, TGA, and nano-indentation mechanical tests. The objective of this study was to assess the impact of these additives on the microstructural, physicochemical properties, including pH-color change sensitivity, and functional properties (antimicrobial and antioxidant activities) of the films for monitoring shrimp freshness.The optical properties were significantly influenced by both ATH and PE, resulting in a substantial enhancement in UV light-blocking capability (approximately 98%) but a reduction in transparency compared to the control film. Also, bionanocomposite films with combined ATH and PE exhibited higher color parameters. AFM revealed a notable increase in film roughness, particularly in PE-rich ternary films. However, the thermal stability was largely unaffected by the incorporation of additives. The occurrence of intermolecular interactions between ATH/PE additives and matrix groups was confirmed by FTIR. Additionally, ATH-included films exhibited pH-sensitivity with visible color changes. Remarkably, ternary films with PE demonstrated improved mechanical properties, reduced moisture content, a lower swelling index, and decreased water vapor permeability with increasing PE content. The addition of 1.5% PE increased the E modulus by 90% and reduced the water vapor

permeability by 66.5% compared to the control film. Importantly, antioxidant assays demonstrated that PE-incorporated films could scavenge DPPH free radicals in a dose- and time-dependent manner, with a maximum inhibition efficiency of 93% observed for ternary films containing 1.5% PE. Moreover, microbiological analysis confirmed the biocidal activities of ternary films against Staphylococcus aureus (S. Aureus) and Salmonella bacteria. Furthermore, ternary films exhibited noticeable color changes during the monitoring of shrimp freshness at 25 °C, with the T-1.5% PE film demonstrating the greatest intelligent response. In conclusion, CMC/Ge-based bio-nanocomposite films developed with intelligent/active functionalities, hold great promise for food packaging applications, particularly in preserving and monitoring the quality of seafood.

Activation, Synthesis and Characterization of Nanocomposite (Cu, Ti-Oxide pillars/Clay)

*Halima Cherifi-Naci[1,2]

1. Research Laboratory of Soft Technology, Valorization, physico-chemistry of Biological Materials and Biodiversity.,L.T.D.V.P.M.B.B, Faculty of Sciences,Boumerdes University, Boumerces, 35000, Algeria.
2. Department of Chemistry, Faculty of Sciences, Boumerdes University, Boumerdes, 35000, Algeria.
cherifi1ch@gmail.com

Abstract:

To expand the scope of clay applications as nanocomposite in several fields, it has become necessary to address the issue of the closure of their slips, speaking to 300 ° C. This disadvantage was overcome by pillaring: Intercalation of cationic complexes of large size, which by calcinations, would turn into pillars oxides which are responsible for the acidity, helped maintain their open structure and create micropores in the interlayer space, thus improving their adsorptive properties. The pillared materials were demonstrated to have an increased interlamellar distance, an increased pore volume and were accessible by molecules within a specific size range. The pillared structure has been suggested to produce acid sites through dehydratation and dehydroxylation of the metal cations at high temperature; the number and strength of the acid sites present in the clay are important factors for exchange and adsorption applications. The effect of attack by sulfuric acid on the physicochemical characteristics of clays is very dependent on treatment conditions (acid concentration, temperature, contact time, pH ...).Considering the importance of the phenomenon of acid activation followed by pillaring operation in the clay applications, we study in this work; activation, synthesis and characterization of modified clay material (nanocomposite), can be used as adsorbent or as acidic catalyst in several organic reactions; The experimental study is to determine the optimal activation conditions (concentration: 5 M at temperature T = 70 ° C, activation time = 4h, adsorbed H_2SO_4 = 1.40 meq / g clay, CEC = 96 meq/100 g clay) to Achieve a adequate activated bentonite aimed to

apply for pillaring operation .Modified clay were characterized by different techniques (XRD, FX) and physic-chemical analysis (CEC: cationic exchange capacity, specific surface area, Average pore diameter and density). Cooper and Titanium pillared material or Cu, Ti-oxides Pillared Clay was synthesized from activated bentonite using $CuCl_2$ and $TiCl_2$ solutions as pillaring agents. The pillared products were characterized by physic-chemical analysis (XRD, CEC, surface acidity, specific surface area, Average pore diameter and volume mass). The basal spacing (d-spacing) for the Cu,Ti-intercalated bentonite and Cu, Ti-pillared bentonite are 39,55 A° and 35 A°, respectively. The specific surface areas of Cu, Ti-pillared and natural bentonites are 370 and 65 m^2 g^{-1} respectively. With specific properties, the complexing clay matrices are highly reactive nanomaterials and can be used in industrial wastewater treatment process or as catalyst in several organic reactions and can be used as resin for dental treatment.

Keywords: Activation, synthesis, characterization, nanocomposite, (Cu,Ti)-oxide pillars.

Method on the physicochemical and catalytic properties of CuAlOx material: Application in the reduction of benzaldehyde reaction

Haddad Naima, Adel Saadi, Axel Löfberg
Laboratoire de gaz naturel, Faculté de Chimie, USTHB
Corresponding author: akrour_naima@hotmail.com

Abstract:
The choice of synthesis method significantly impacts the physicochemical properties of materials, even with identical compositions, making it crucial for precise catalytic applications. Parameters such as crystallinity, homogeneity, morphology, and dispersion can be altered accordingly.
In this regard, We synthesized bimetallic oxide Cu-Al-O (Cu/Al=1) using the sol-gel method (designated CuAl-SG) and compared it with the hydrothermal system (CuAl-Hyd). Both systems were thermally treated under N2 at 500°C and characterized using XRD, BET-BJH, and SEM techniques. Catalytic activity was assessed in the reduction of benzaldehyde within the 150-200°C temperature range. The XRD comparison of CuAl-Hyd and CuAl-SG systems reveals the influence of the preparation method on the structural properties of Cu-Al-O. While the hydrothermal system forms CuO and Al2O3 oxides, the sol-gel method produces CuAlO2 with a hexagonal delafossite structure. The preparation method also affects the textural properties of CuAl. Porosity results show a significant difference, with the specific surface area of CuAl-Hyd being 80% larger than CuAl-SG (106 m2/g vs. 22 m2/g). The BJH analysis indicates a more homogeneous pore distribution in the sol-gel system, characterized by two peaks representing different pore sizes. SEM imaging highlights distinct morphologies between CuAl-SG and CuAl-Hyd, with the former displaying uniformity and particle agglomeration. Additionally, CuAl-Hyd exhibits smaller particles with uniform size distribution and lower crystallization degree.

CuAl-SG demonstrates superior reactivity in benzaldehyde reduction, with enhanced conversion (3% to 28% and 54% to 79%) and selectivity towards benzyl alcohol (0% to 46% and 0% to 34%) at 150 and 200°C. The copper oxidation state (+I) in CuAlO2 favors the activity of CuAl-SG. Furthermore, the sol-gel system's homogeneous pore distribution and small pore volume with a high average diameter may facilitate benzylate species desorption, enhancing selectivity towards benzyl alcohol.

Electrochemical study of elaboration of nickel manganese alloy

Hizia Merkoune and Kamel Hachama
University of Djillali Bounaama Khemis Miliana
Corresponding author: merkoune.hizia@gmail.com

Abstract:
Many applications are offered from materials nickel and manganese are used because of their catalytic power in several reactions like electrolysis of water with give two important element for life hydrogen and oxygen.
Our work is short study of electrodeposition of nickel and manganese explained in voltamigramms and the effect of PH on the kinetic of the behavior elaboration.

Dry Reforming of Methane over Ni/Al/Fe catalysts derived from hydrotalcites

Baya Djebarria[2], Fouzia Touahra[3], Nadia Aidera[4], K.Debaah[1], Khaldoun Bachari[3] and Djamila Halliche[1].

[1]*Laboratory of Natural Gas Chemistry, Faculty of Chemistry, USTHB*

[2]*Lab-CAM, University of M'hamed Bougara of Boumerdes, Algeria*

[3]*CRAPC, BP 384-Bou-Ismail-RP42004, Tipaza, Algeria.*

[4] *LCAGC, Mouloud Mammeri University of Tizi-Ouzou, Algeria*

Corresponding author: b.djebarri@univ-boumerdes.dz

Abstract:

Bimetallic Ni-Al and Ni-Fe nanoparticles catalysts drived from hydrotalcite were synthesized by co-precipitation method and applied in dry reforming of methane. The samples were calcined at 800 °C and the crystalline phase was assessed by XRD coupled with Rietveld refinement. Other analyzes were carried out to study their textural and structural properties including, Thermogravimetric Analysis, Coupled Plasma Atomic Emission Spectroscopy, Brunauere-Emmette-Teller, SEM and EDS, Temperature Programmed Reduction, TEM and EDS mapping. These catalysts were evaluated in CO2 reforming of methane under continuous flow with CH4/CO2 ratio equal to 1, at atmospheric pressure and a temperature range between 400 °C and 700°C. At 700°C, the NiAlHT catalyst displayed the best CH4 conversion (87.5%) and CO2 conversion (91.4%) compared to conversion of CH4 (79.2%) and CO2 (84.1) for NiFeHT catalyst within 10 h stability test. The iron addition to the nickel showed improved resistance to coke deposition while a slight decrease in methane conversion was observed. The possible formation of □-NiFe alloy observed during the study of reducibility by hydrogen was invoked to account for the catalytic behavior.

Keywords: Hydrotalcite, Greenhouse effect, Ni-Fe alloy, Synergistic Effect in Bimetallic, reforming methane with CO2.

Identification of the active species of keggin-polyoxometalates in the oxidation reaction of cyclohexanone

D. Amitouche, I.Sebai, S.Mouanni, Tassadit Mazari, Mohamed Haouas, C. Roch.Marchal and C. Rabia
Chemical Engineering and Applied Chemistry Laboratory (LCGA). UMMTO, Tizi Ouzou 15000, Algeria.
Corresponding author: dahbia.amitouche@ummto.dz

Abstract:
Polyoxometallates of the Keggin structure based on zinc with the formula H3-2xZnxPMo12O40 (H3-2x Znx) (with x: 0-1.5) have been prepared, characterized by several physico-chemical analyses, then investigated in the reaction oxidation with 30mmol -One, 1% (30mg) of catalyst, at 90 ° C, using H2O2 (30%) as green oxidant. A sequenced addition of 0.5ml of H2O2 (30%) was made every 30 min. The catalytic process of the oxidation was examined in situ by multinuclear NMR (31P, 95Mo, 17O) and by UV-Visible in order to follow the evolution of the catalyst during the reaction and to determine the active species.The catalysts have shown good activity and the purties of AA was invistigeted by 1H and 13C NMR. At the end of the reaction, the identification of the products and by-products is carried out spectroscopically via 1H, 13C, 1H-1H (Cosy) NMR and MS.

Extractions and experimental studies of citrus sinensis extracts as an economic and ecological corrosion inhibitor for mild steel in hydrochloric acid medium

Bouchhit chaima , Boudinar Yamina, Hammouda Nadia, Bounedjar Nourelhouda, Seniguer Amel, Fares Ali

University 20 August 1955- Skikda - Faculty of Science - Chemistry department

Corresponding author: ch.bouchhit@univ-skikda.dz

Abstract:

Green corrosion inhibitors are of great interest because of their exciting and environmentally friendly behavior in controlling mild steel corrosion in different aggressive media. Citrus sinensis extract «bark and leaves» could be cost-effective and effective inhibitors. In this work, the leaves and barks of CS were successfully extracted, and they were characterized by qualitative chemical tests and spectroscopic measurements. Extracted CS were tested as green inhibitors for the MS corrosion in a 1.0 M HCL. The inhibition efficiency of CS extract against corrosion of mild steel A37 was evaluated by electrochemical (PC) and EIS methods. In addition, the adsorption isotherm, free adsorption energy and thermodynamic process parameters were evaluated. Electrochemical tests showed good inhibitory efficacy at an optimal concentration of 2000 ppm to 73% in the case of bark. Open circuit potential (OCP) and potentiodynamic polarization results indicated that the extracted CS acted as a mixed type of inhibitor. The inhibitors act by adsorption on the surface of the steel, the values of the thermodynamic parameters for the adsorption of inhibitors can provide valuable information on the mechanism of corrosion inhibition. Based on the results, it is revealed that citrus sinensis (E, F) extracts can serve as an excellent green, ecological and promising inhibitor against corrosion of mild steel.

Metallic nanoparticles growth on ionic layer grafted onto glassy carbon for hydrogen evolution reaction

Hocine Moussouni, Mourad Mechouet, Jalal Ghilane
LPCM, University of Mouloud Mammeri, Tizi Ouzou, Algeria
Corresponding author: hocine.moussouni@fs.ummto.dz

Abstract:
In this work, we focused on the electro-grafting of thin film based on ionic liquids (LIs) on a glassy carbon electrode (GC), then functionalized with metal nanoparticles (Pt or Pd). The XPS obtained spectrum confirm the modification of the electrode. Interestingly, the catalytic performances of hydrogen evolution reaction (HER) are improved for both prepared electrodes (GC/LI/Pt, GC/LI/Pd), especially the latest one containing palladium which present the best electrocatalytic activity towards HER, better than the commercial platinium Pt/C considered as reference material for this type of reaction . It seems that the presence of the ionic layer displays an increase catalytic, which is probably due to the synergistic effect existence between the grafted ionic layer and the metallic nanoparticles.

Improvement of structural and optical properties of monolike(quasi-monocrystalline)silicon wafers by chemical treatment

G. Benseba, A. Moussi, D. Hocine, D. Salem
Advanced Technologies Laboratory of electrical engineering (LATAGE), University Mouloud Mammeri of Tizi-Ouzou (UMMTO)
Corresponding author: ghalia.benseba@ummto.dz

Abstract:
In this work we studied the silicon monolike (ML-Si) material. Its structural and chemical properties are analyzed and compared to those of Czochralski-monocrystalline silicon (Cz-Si) and multicrystalline silicon (mc-Si). The reflection properties of alkaline-etched wafers were investigated using UV-VIS-NIR spectrophotometer and the images of the surface morphology were obtained using a scanning electron microscope (SEM) recording spectra (EDX) and Atomic Force Microscope (AFM) was performed to determine the surface roughness. We observe that Cz-Si and ML-Si present the same morphology. Reflectivity of ML-Si is 5% higher than that of Cz-Si and much lower than mc-Si surface after NaOH texture.
We also note that ML-Si is almost identical to Cz-Si. The ML-Si with favorable morphological and optical properties are indeed promising for photovoltaic (PV) applications.
This research could potentially lead to advancements in solar cell technology and other fields where high-quality silicon materials are utilized.

Keywords: Mono-Like silicon; quasi-monocrystalline silicon ; chemical treatments; analysis; texturing.

Selectivity study of Bi2Fe4O9/Ag3PO4 catalyst

Adel Khen, Toufik Hadjersi, Madjid Ifires
Centre de recherche en technologie des semi-conducteurs pour l'énergétique (CRTSE)
Corresponding author: adelkhane@gmail.com

Abstract:
In this work, the selectivity of Bi2Fe4O9/Ag3PO4 toward organic pollutants was investigated. The composites were prepared via hydrothermal and precipitation method. The obtained composites were characterized by scanning electron microscopy (SEM), X-ray diffraction Photoluminescence (PL) and UV-Vis spectrophotometry. The Bi2Fe4O9/Ag3PO4 catalyst exhibited the high photocatalytic performance toward rhodamine B (RhB) with degradation efficiency of 97.91 % after 12 min under visible light irradiation. The photodegradation rates of methylene blue (MB) and tartrazine were 94.34 %, 94.48 within 12 min of visible light irradiation. The cycling experiment revealed that Bi2Fe4O9/Ag3PO4 catalyst has a good stability after 4 runs.

Catalytic decomposition of n-butanol over catalysts prepared from cexmny-Mg4Al2 hydrotalcite-like compounds

Naima Haddad, Faiza Sahraoui, Jean-François Lamonier
Laboratoire de gaz naturel, USTHB
Corresponding author: akrour_naima@hotmail.com

Abstract:
Industrial processes release a plethora of volatile organic compounds (VOCs) into the atmosphere, which adversely affect human health and contribute to air pollution, smog formation, and the degradation of urban air quality. Certain VOCs are also linked to climate change as they have the ability to trap heat in the atmosphere. To tackle this issue, catalytic oxidation has emerged as a promising solution for the complete elimination of VOCs. In this context, our study investigates Ce and Mn-containing MgAl LDH, focusing on its structural and catalytic properties. The Mn_XCe_Y-Mg_4Al_2-HT systems (with x = 0, 0.4, 0.6, and 0.8 and x+y=0.8) were prepared using a two-step calcination-reconstruction process. The effects of Ce and Mn content on the structural and catalytic properties of Ce and Mn-containing MgAl LDH were investigated. The samples underwent characterization using XRD, BET, Raman, XPS, and ATG techniques. The catalytic activity of the resulting compound in n-butanol oxidation was examined. Increasing Ce and/or Mn contents led to changes in the structural, textural, and reducibility properties of the synthesized systems. The catalyst with high Ce content exhibited the highest catalytic activity. Conversely, the addition of a low amount of Mn to the system (Ce0.6Mn0.2-Mg4Al2) significantly improved CO2 formation. The formation of active sites occupied by cerium and manganese within the LDH structure, contributed to the material's performance. The Ce3+/Ce4+ and Mn3+/Mn4+ redox couples in the external layers enhanced O2- diffusion and their activation into nucleophilic species, facilitating butanol transformation.

First-principle study of the structural, mechanical, and electronic properties of orthorhombic CH3NH3SnI3

Amina Dendane, Benali Rerbal
University ABOU BAKR BELKAID TLEMCEN
Corresponding author: dendaneamina@yahoo.com

Abstract:

CH3NH3SnI3 is a nanomaterial with great potential for high-performance photovoltaic applications. It stands out as a fascinating example of a nanomaterial particularly well-suited for sustainable environmental and energy applications.

This material boasts high energy conversion efficiency, along with a relatively simple and cost-effective synthesis method, making it a prime candidate for photovoltaic devices. Additionally, the abundant availability and non-toxic nature of its components significantly contribute to reducing the environmental impact of the production and use of solar cells based on this material

With a direct band gap and a flexible structure, our study aims to deepen the understanding of the energy stability of CH3NH3SnI3 in its orthorhombic structure using first principles. Using the VASP code, we are exploring its mechanical and electronic properties, paving the way for new applications in the field of sustainable energy. This research is part of an innovation and sustainability approach aimed at making significant advances in the field of nanomaterials for renewable energies.

Production of Catalytically Active Lead from Lead Sulfide for Electrochemical Reduction of CO2 into Formate

Chahinez Ahmed Ouamer, Ibtissem Chibane, Samira Kaci, Lamia Talbi, Karima Benfadel, Sabiha Anas Boussaa, Assia Boukezzata, Yahia Ouadah, Oussama Djemaa, Djaouida Allam, Sihem Aissiou Bouanik, Toufik Hadjersi

CRTSE, Algeria

Corresponding author: kacisamirahdr@gmail.com

Abstract:

The presented approach offers a methodology for synthesizing lead nanoparticles from the sulfide (PbS) and subsequently using them as catalysts for electrochemical CO2 reduction. The simplicity of the synthesis process and the stability of metal sulfide nanoparticles make this method particularly appealing. Various characterization techniques, including XRD, SEM, EDX, and XPS, were utilized to analyze the structure, morphology, bulk, and surface compositions of the catalyst before and after reduction. Formate production rates were measured at potentials of -1.8 and -2.0 V vs Ag/AgCl, with the highest rate observed at -2.0V.

Electrochemical evaluation and structural characterization of Graphite surfaces modified with PbS for CO2 electroreduction to HCOOH

Ibtissem Chibane, Chahinez Ahmed Ouamer, Samira Kaci, Lamia Talbi, Karima Benfadel, Sabiha Anas Boussaa, Assia Boukezzata, Yahia Ouadah, Oussama Djemaa, Djaouida Allam, Toufik Hadjersi
Centre de recherche en technologie des semiconducteurs pour l'énergétique

Corresponding author: kacisamirahdr@gmail.com

Abstract:
Graphite was modified with nanoparticles of lead sulfide (PbS) to enhance its electrochemical performance towards CO2 electroreduction. The surface characteristics, crystalline structure, and electrochemical behavior of the graphite/Pb-based electrodes were analyzed and compared with pristine graphite. Surface modification was found to enhance the current density without compromising its specific stability. The electrochemical properties of the synthesized graphite/PbS electrode were assessed using cyclic voltammetry (CV) and AC impedance techniques in 0.5M NaOH electrolyte. An enchantement in specific capacitances were achieved for graphite and graphite/PbS, respectively. This enhancement is attributed to the synergistic effect of Pb2+ ions in thé graphite/PbS electrode.The resulting graphite/PbS nanocomposite displayed highly stable and porous layered structures. This study underscores the favorable structural stability and electrochemical performance of graphite/PbS nanomaterials, positioning them as promising materials for CO2 electroreduction application.

Elaboration and application of PbS/C/PVDF nanocomposites-based electrodes for CO2 electrochemical reduction to HCOOH

Samira Kaci, Chahinez Ahmed Ouamer, Ibtissem Chibane, Lamia Talbi, Karima Benfadel, Sabiha Anas Boussaa, Assia Boukezzata, Yahia Ouadah, Toufik Hadjersi

CRTSE, Algeria

Corresponding author: kacisamirahdr@gmail.com

Abstract:

The surface of a carbon-supported cathode, containing lead sulfite and carbone nanoparticles, facilitates the selective electrochemical conversion of CO2 to HCOOH. Traditional lead sulfide catalysts tend to produce lead oxide under certain conditions, but by modifying lead sulfide with varying amounts of PVDF, we synthesized cathodes optimized for converting CO2 into formic acid. Through our targeted preparation method, we established a relationship between metal content and catalytic activity, achieving a Faradaic efficiency of around 70% for formate formation at -2 V vs. Ag/AgCl, representing a 450 mV overpotential at pH=10. This reduction reaction reduces the simultaneous production of H2, while the presence of lead nanoparticles enhances activity and efficiency by directing the CO2 reduction towards formate rather than carbon monoxide or H2 evolution.

Synthesis and characterization of a new supported copper nanomaterial: application in removal of methylene blue dye

Ouardia Zekri, Thiziri Djelloudi
USTHB, Algeria
Corresponding author: ouardiazekri@yahoo.fr

Abstract:
Nowadays, there are a number of different sectors, such as pharmacy, textile, food, paper, leather, batteries, rubber, cosmetics and plastics, which still releasing their effluent discharges into the neighboring ecosystems. These effluent discharges contain toxic and carcinogenic substances, affecting significantly the groundwater quality, the natural environment, and human health . The dyes present a major source of water contamination. Consequently, the degradation of these dyes from wastewater has been carefully investigated. In this work, 2%Cu/SiO2 nanocatalyst was elaborated by wet impregnation method. This as-synthesized material was characterized by XRD, FTIR, TGA, BET and FRX analysis. The efficiency of the prepared catalyst was tested in the removal of methylene blue dye (MB) as a model of textile contaminants by adsorption. The effect of various operational factors such as initial pH, adsorbent dose, methylene blue concentration were investigated. A total removal of the dye was reached rapidly. After regeneration (up to three cycles), the catalyst showed high stability.

Key words: Copper, adsorption, MB, nanomaterial.

Synthèse et étude structurale d'un complexe de coordination à transition de spin

Seniguer Amel, Boudinar Yamina, Ait Ramdane Chafia, Setifi Zouaoui, Bounedjar Nourelhouda,Bouchhit Chaima, Fares Ali
Faculté de Science Département Chimie
Corresponding author: amelseniguer1997@gmail.com

Abstract:
Studies of bistable molecular materials have grown in recent years due to their many potential applications in the fields of molecular electronics and switching. In this context, nitrile anions represent a very good ligands in the design of new molecular materials with spin transition phenomena and various structures.
In this work, the association of the monoanion NCS- with the neutral co-ligand abpt (4-amino-3,5-bis (pyridin-2-yl) -1,2,4-triazole) led us to obtain a new phase of formula [Fe (abpt) 2 (NCS) 2] which exhibits a gradual spin transition with a temperature T1/2 of 162 K."

Synthesis of hydroxyapatite and application to textile dye adsorption

Kahina Annane, Hocine Grabi, Ouahiba Hocin1, Wahiba Lemlikchi et Slimane Kadouche
UMMTO, Algeria
Corresponding author: kahina.annane@ummto.dz

Abstract:
In the present study, hydroxyapatite (HAp) was synthesized and applied to remove solophenyl blue (BS) dye from an aqueous solution. The physicochemical properties of HAp were characterized by infrared spectroscopy and BET method.
Several parameters have been optimized: initial pH, mass of the adsorbent, initial concentration of the dye, contact time and temperature to remove the dye from an aqueous solution. Adsorption kinetics showed that equilibrium is reached after 40 minutes with a removal efficiency of 98.5% for an adsorbent mass of 0.06 g at pH=6.
Kinetic and isothermal studies showed that the adsorption of BS followed the pseudo-second order model and the Langmuir isotherm was found to be the most appropriate model.
The thermodynamic study revealed that the adsorption is spontaneous, endothermic and physical in nature.

Key words: Synthesized hydroxyapatite, solophenyl blue, adsorption.

Study of hydrogen bonds using Bernstein's theory of two copper-based hybrid materials

Rakhoum Youcef, Damous Maamar, Belhocine Yougharta, Allal Hamza, Hamlaoui Meriem
Université 20 août 1955 skikda
Corresponding author: rakhoumyoucef8@gmail.com

Abstract:
The synthesis of new hybrid materials formed from copper and organic matrices based on oxygenated and nitrogenous ligands has experienced significant growth in recent decades. The 2-hydroxy-1-naphthaldehyde ligand attracted our attention because it showed enormous potential in terms of complexation with metallic centers. The aqueous synthesis of compounds based on copper and organic matrix gave two new compounds which are:
1- bis(2-oxy-1-naphthaldehyde-O,O')-copper(II).
2-(1,10-phenanthroline)-(2-oxy-1-naphthaldehyde-O,O')-(dimethylsulfoxide)-copper(II) perchlorate.
The structural study and physicochemical characterization of these two compounds was carried out using two techniques, namely single crystal X-ray diffraction and differential thermal analysis. The study of hydrogen bonds based on Bernstein's theory made it possible to explain the cohesion of molecules in the crystal.

Key words: Oxygen ligand, nitrogen ligand, hybrid materials, X-ray diffraction, thermal decomposition.

The Synergistic Effect of a new organic compound on the corrosion behavior of carbon steel in hydrochloric acid: Experimental and Molecular dynamics simulation study

Sonia Benabid, Rahma Amina Rikouh, Houria Debab, Hanane Hamani, Tahar Douadi

Laboratory of Electrochemistry of Molecular and Complex Materials (LEMMC), Department of Process Engineering, Faculty of Technology, Setif-1 University-Ferhat ABBAS, Setif, Algeria

Corresponding author: sonia_benabid@yahoo.fr

Abstract:

The inhibition and synergistic effect of a new organic compound (PAHP) with KI on the corrosion of carbon steel in 1.0 M HCl solution were investigated by potentiodynamic polarization technique. The results showed that, with the addition of 5x10-4 M of potassium iodide, the inhibition efficiency of 5x10-4 M of PAHP has been improved from 76, 82% to 84.41%. Photographs obtained by optical microscope affirmed the formation of protective film on carbon steel surface. The influence of molecular configuration in corrosion inhibition behavior of PAHP inhibitor has been explored by Molecular dynamic simulation.The results given by the MD simulation are in good agreement with the experimental results.

Key words: corrosion, synergism, optical microscope, MD simulation.

An investigation into the corrosion inhibition mechanisms of mild steel using Schiff base in an acidic environment

Hanane Hamani, Sonia Benabid , Houria Debab , Tahar Douadi
Department of Génie des Procédés, Faculty of Technologie, University Saad dahleb, Blida- Algérie
Corresponding author: hanane.hamani@gmail.com

Abstract:
Corrosion of metals, particularly mild steel (MS), poses significant challenges in multiple industries, causing economic losses, structural deterioration, and safety issues. Traditional corrosion prevention methods, such as synthetic coatings and alloying, have limitations in terms of cost, environmental impact, and effectiveness. Our objective was to gain enhanced insight into the corrosion inhibition behaviour of mild steel rods when immersed in an acidic solution. The chosen acidic environment was intentionally designed to replicate the corrosive conditions prevalent in both industrial processes and natural environments.
The corrosion behavior of mild steel in 1M HCl solution in the absence and presence of newly Schiff base was investigated using electrochemical impedance spectroscopy (EIS), Potentiodynamic polarization and scanning electron microscopy (SEM). All the experimental results show that these Schiff base have a good corrosion inhibition performance. The polarization curves show that these compound act as mixed-type inhibitors. The adsorption of these Schiff base on carbon steel surface is consistent with Langmuir adsorption isotherm. DFT calculation and molecular dynamic simulations were in excellent agreement with the experimental tests.

Keywords : Corrosion inhibitor; mild steel; hydrochloric acid; polarization

Orange II degradation using LaCoO3/ZnO hetero-system under solar light

Ouatizerga Abdelaziz, G. Rekhila, S. Mirad, M. Trari
Faculty of physics – USTHB, Algeria
Corresponding author: ouabdela@gmail.com

Abstract:
LaCoO3 elaborated by nitrate route was characterized physically and electrochemically to be applied in the Orange II (OII) oxidation upon solar light. The XRD analysis showed that the single phase is completed at 850 °C and the oxide crystallizes in a distorted perovskite structure. The peak at 643 cm-1 in the ATR spectrum confirmed the purity of the phase. The forbidden band (1.35 eV), determined from the diffuse reflectance is assigned to Co3+: d-d transition. The thermal variation of the conductivity is characteristic of non-degenerate behavior and a holes mobility of 10-2 cm2V-1s-1 and an activation energy of 0.11 eV. The latter is different from that obtained from the thermo-power, a signature of a conduction mechanism by small polaron hopping. An exchange current density of 40 μAcm-2, a polarization resistance of 1.92 kΩ cm2 and a corrosion potential of 0.99 VSCE were obtained at pH ~7. The variation of the inverse of the square of the capacitance as a function of potential indicates p type behavior with a flat band potential of 0.30 VSCE and holes density of 1.97×1017 cm-3. The conduction band (-0.94 VSCE), made up of Co3+: 3d orbital, enables the formation of the radical O2•- and as application, the oxide was successfully experimented for the oxidation of OII. The hetero-junction LaCoO3/ZnO enhances the photo-activity due to the facile transfer of electrons with an abatement of 86% at neutral pH. The oxidation follows a first-order kinetic with a half photocatalytic life of 23 min.

Comparative study between single rod and multi rods approach for Nd :YAG active mediums in solar laser side pumping configuration based on off axis parabolic mirror (OAPM)

Imene Kouicem, Saïd Mehellou, Raguig Maroua, And Ferhat Rehouma

LEVRES Laboratory, University of El Oued, 39000 El Oued, Algeria

Corresponding author: kouicem96@gmail.com

Abstract:

Solar lasers are an emerging technology of lasers that utilize solar energy, as it is the most plentiful type of energy, to convert the sun rays featured by a broadband spectrum to produce narrow-band laser radiation. This innovative approach holds immense potential for various applications across diverse fields, ranging from scientific research and industrial manufacturing to telecommunications and space exploration, such as wireless power transmission, deep-space optical data transmission, and asteroid deflection…etc. In this study, a comparative study performed by Zemax ray tracing software to explore the effeciency of side pumped Nd:YAG active medium in both single and multirod configurations within a laser system based on two off-axis parabolic mirrors (OAPM), an absorbed energy of 74.4 w is obtained when using a single thick rod of 8 mm diameter and 48 mm length, while an absobed energy of 76.697 w is acquired when using three thinner rods of 5.2 mm diameter and 48 mm length for each one, which emphasizes the enhancing role of the multirod approach in producing higher absorption effeciency and theraby more stable output power laser.

Key words: solar laser, Nd:YAG, OAPM,multi rods , sun pumped laser.

Preparation, Charactirisation of Kigging Phosphotungstic Acid Supported on Silica, Polyacrylamide Hydrogel for Methanolysis Reaction

Toumi Feriel, Idrissou Yasmina, Mazari Tassadit
LCAGC, Faculty of chemistry, University of Mouloud Mammeri TiziOuzou
Corresponding author: feriel.toumi@ummto.dz

Abstract:
The catalytic activity of 12-tungstophosphoric acid (HPW) in homogeneous and heterogeneous systems was evaluated for oleic acid and cooking oil esterification in presence of methanol (methanolysis), with an fatty acid/methanol ratio of 1/9, a reaction temperature of 60 °C and a reaction time of 3 h.
Heterogeneous catalytic systems based on phosphotungstic acid catalyst (HPW) supported on silica, polyacrylamid hydrogel (PAAm) and polyacrylamide/ β-cyclodextrin noted respectively (SiO2/HPW), (PAAm/HPW) and ((PAAm/ β-CD)/HPW) are obtained with different amount of HPW (10-30 wt%). The insertion of HPW and β-CD in polyacrylamid was carried out with different methods. The main of this work is to determine the yield of biodiesel by proving the materials catalytics performance in esterification reaction.
The catalytic materials were characterized by FTIR and the fatty acid methyl esters, reaction products, were analyzed and quantified by gas chromatography. The swelling behavior of materials (HPW/PAAm) and ((PAAm/(β-CD)/HPW) was studied in distilled water at 25°C, and in fatty acid /methanol at 25 and 60°C which simulates the reaction medium.

Physical characterizations of silver pyrophosphate (Ag4P2O7) and orthophosphate (Ag3PO4). MO degradation under visible and solar lights

Razika Brahimi, Yasmina Keriti, Mohamed Trari
Faculty of Chemistry, USTHB, Algeria
Corresponding author: razikabrahimi@gmail.com

Abstract:
This work is devoted to physical characterizations of Ag4P2O7 and Ag3PO4 such as X-ray diffraction, diffuse reflectance, ATR and electrochemical analysis. Their band diagrams were established in order to predict the feasibility of photocatalytic reactions at their interfaces. In this regard, methyl orange (MO) was used as a model pollutant, it was degraded at the interface of the both materials under solar and visible lights. The experimental results have undoubtedly demonstrated that the most photoactive material was indeed Ag3PO4 with a degradation efficiency of 99% for 50 min under visible light.

Photocatalytic degradation of the AG25 dye by CaFe2O4 nano particles synthesized using green chemistry method

Fatiha Abdelmalek, Batoul Benidriss, Sabri Khalifa, Rachida Bendahman, Ahmed Addou

Laboratory of Environmental Science and Valorization, Department of Process Engineering, University Abdelhamid Ibn Badis Mostaganem, BP 188, 27000 Mostaganem, Algeria

Corresponding author: salima.daoui.etu@univ-mosta.dz

Abstract:

CaFe2O4 nanoparticles, synthetised by green chemistry using sol-gel auto-combustion, from carob leaves were used for the removal of AG dye in aqueous solution. Characterisation was carried out by X-ray powder diffraction, scanning electron microscopy coupled to energy dispersive X-ray spectroscopy, Fourier transform infrared spectroscopy and Raman spectroscopy.

The characterization techniques based on X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and Raman spectroscopy showed that the NPs crystallize in the spinel cubic system Fd-3m (o_h^7). The application of these nanoparticles for the photocatalytic degradation of AG25 was studied by varying the following parameters: catalyst quantity (0.1; 0.2; 0.5; 0.75 and 1 g/L),, dye concentration ((37.5, 75 and 100 µM),), pH (2; 6.7 and 8), and exposure time to visible light (5; 10; 20; 30; 45 and 60 min). Optimization of several parameters based on experimental design, such as catalyst quantity, dye concentration, solution pH, and exposure time, was conducted. The results showed that at pH 2, with a catalyst quantity of 0.25 g/L, dye concentration of 37.5 µM under a 100W LED visible light bulb, and within 20 minutes, 97% of AG25 was degraded.

Insulating Nano-liquids Assessment Using the Conduction Currents Technique

Abdeslem Beldjilali
Material Physics Laboratory, USTHB, Algeria
Corresponding author: abdeslembeldjilali@gmail.com

Abstract:
Nano-fluids technique, involve the controlled dispersion of nanometric particles in dielectric liquids, has proven effective in enhancing insulation performance. In this context, this study investigates the electrical insulation capabilities of nano-fluids based on Algerian vegetable olive oils. The nano-dielectric liquid under study is prepared by dispersing FeAl2O3 nano-particles in olive oil at a concentration of 0.01g per liter. Electrical response measurements of the olive oil nano-fluid samples are conducted under various DC electric fields, ranging from 30 to 150 Volts, applied to a nano-liquid with a thickness of 0.2mm. Considering the diverse operational conditions of power transformers, three types of samples are analyzed using polarization and depolarization current measurements: FeAl2O3 particles in virgin olive oil, FeAl2O3 particles in aged olive oil, FeAl2O3 particles in olive oil aged in the presence of cellulose material. The results reveal that the local olive oil exhibits acceptable compatibility as a suitable matrix for nano-insulating materials. Specifically, the recorded electrical currents under DC fields range within a few nanoAmperes. Moreover, the observed evolution of electrical current with increasing electric field strength suggests a quasi linear behavior, while the relaxation currents, measured after removing the electrical constraints, lack specific characteristics. This absence of polarization indicates that electrical charges carriers do not accumulate within this type of insulating system.

Key words: Conduction currents, Nano fluids, olive oils.

Study on the effectiveness of CoFe2O4 nanoparticles for degrading the organic pollutant AG25 in an aqueous medium via an advanced oxidation process.

Fatima Zohra Benkrifa, Fatiha.Abdelmalek, Kalifa.Sabri, El Batoul.Benidris, Chaimaa.Hachemi, Ahmed.Addou

Laboratory of Evironmental Science and Valorisation, Department of Process Engineering, University Abdelhamid Ibn Badis Mostaganem, BP188,27000 Mostaganem, Algeria.

Corresponding author: fatimazohra.benkrifa.etu@univ-mosta.dz

Abstract:

In this study, cobalt nano-ferrite CoFe2O4 (NFCo) was synthesized using the sol gel self-combustion method. Structural (XRD, FTIR and Raman), morphological (SEM with EDAX) and magnetic (VSM) properties were characterized. XRD analysis revealed the formation of a pure phase with a mixed spinel structure and an average crystallite size of 60 nm. SEM observations revealed the existence of particle agglomerates and a porous morphology. FTIR analysis identified characteristic M-O vibrational peaks at the tetrahedral and octahedral sites, with the Raman study confirming the spinel structure. Magnetic analysis revealed that the coercive field increased resistance to demagnetization. Various oxidation processes, including UV, plasma-activated water (PAW) by gliding arc discharge (GAD), NFCo, as well hybrid UV, PAW/UV, NFCo/UV, PAW/NFCo and PAW/NFCo/UV systems, were used to assess the removal of the AG25 dye. Removal processes, mechanisms and photocatalysis were studied. Optimal conditions for efficient removal were identified for all processes studies.

Keywords- PAW, CoFe2O4, POA, AG25, photocatalysis

Visible-Light-Driven Photocatalytic Degradation of Methyl Violet by Zn and Ni Doped TiO2

Nabila Bouabdallah, Madani Ghelamallah

Laboratory of Environmental Science and Valorization(STEVA), Department of Process Engineering, Faculty of Science and Technology, University Abdelhamid Ibn Badis Mostaganem,27000 Mostaganem, Algeria.

Corresponding author: nabila.bouabdallah.etu@univ-mosta.dz

Abstract:

The contamination of water has been an important issue for environmental scientists in last decades. The waste water of the textile factories is known to contain a large amount of different azo dyes and salts. Methyl Violet (MV) has been identified as one of the most problematic dyes, present in the industrial effluents, which can be potentially life threatening for living organisms. Therefore, its detection and elimination are challenging goals.

Titanium oxide (TiO2) doped by Zn and Ni have been synthesized through a sol gel method.

The catalysts thus obtained were characterized by the BET specific surface area method and Uv-Visible spectroscopy for solid. BET results showed that the addition of Zn increased the specific surface area of TiO2, while Ni had a negative effect. A significant lowering of Eg can be observed on the Ni-TiO2 catalyst. TiO2 doped by Zn enhanced the photocatalytic activity compared to Ni-TiO2. The photodegradation of Methyl violet was investigated from a synthetic solution with a concentration equal to 5 mg/L for a mass of 0.05g of catalyst. Degradation capacities were reached up to 7.15, 7.40 and 1.98 mg/g for TiO2 alone and TiO2 modified with Zn and Ni, respectively.

Keywords: Photocatalysis; Methyl violet; TiO2; light irradiation; Sol-gel

Application of phosphomolybdic acid nanomaterial in the heterocyclessynthesis

Fella Gaad [1,2], Sabrina Halit [1], Malika Makhloufi [1], Tassaditmazari [2], Catherineroch Marchal[3]

[1]*LPCM, University of Mouloud Mammeri,Tizi-Ouzou, Algeria.*

[2]*LCAGC, Université Mouloud Mammeri Tizi-Ouzou, Algeria.*

[3]*Institut of Lavoisier (ILV), Versaillesuniversity, Saint quentin in Yvelines*

Corresponding author: fella.gaad@ummto.dz,

Abstract :

The application of heteropolyanionic nanomaterials (HPA) in the synthesis of heterocyclic nitrogen compounds is the main subject of this study. Indeed, dihydropyridines (DHPs) occupy an important place in the medicinal chemistry. They have been widely used as fundamental building blocks in drug development. On the other hand, the research and development of catalytic nanomaterials allowing ecological and sustainable access to DHPs, which can overcome the constraints of conventional processes such aslong reaction time, low yield, the use of hazardous reagants, the solventstoxicity, is of capital importance. Thus, heteropolyanions can acts as potential candidates to meet these requirements, in fact, they are bifunctional, easy to prepare, clean and efficient, and above all, can be used either in homogeneous or heterogeneous environment, which explains our choice. A parametric study of the DHPs production reaction in the presence of the phosphomolybdic heteropolyacid as parent catalystpermitted us to identify some optimaloperational conditions. At the last, the purity of the synthetised products and the reliability of the chosen process were verified by various analytical techniques.

Keywords: $H_3PMo_{12}O_{40}$, HPAs nanomaterials, green chemistry,heterocycles, DHPs, catalysis.

Elaboration and photocatalytic properties under visible light irradiationof cu2o coated silicon nanowire arrays

Mahmoudi Meriem, Hadjersi Toufik
University of Blida 1
Corresponding author: meriemmahmoudi4@gmail.com

Abstract:
In this study, a simple and low-cost chemical method was used to synthesize a new generation of photocatalyst namely Cu2O-modified silicon nanowires (SiNWs). These new heterogeneous photocatalysts were used for degrading of Malachite Green in aqueous medium under visible light irradiation. SiNWs were elaborated by a one-step Ag-assisted chemical etching of the silicon substrate in an aqueous solution of HF and AgNO3. SiNWs/Cu2O nanoheterojunctions were prepared using an electroless deposition technique to deposit Cu2O nanocrystallines on the surface of SiNWs. The prepared samples were characterized by scanning electron microscopy (SEM) which showed that silicon nanowires were uniformly formed on the whole surface and regularly oriented in the perpendicular direction to the sample surface. The unmodified silicon nanowire X-ray diffraction pattern (XRD) exhibits a high intensity peak relative to the presence of silicon (Si). The photodegradation of Malachite Green (MG) using modified and unmodified silicon nanowires as photocatalysts was evaluated by measuring the decay of absorption peak every 10 min of visible light irradiation for 100 min. The results obtained showed that Cu-modified silicon nanowires have the highest performance in terms photocatalytic efficiency compared to unmodified SiNWs where they allowed degrading of about 99% of MG after visible light irradiation 100 min.

Keywords: Siliconnanowirearrays, Copper oxide, Malachite Green, Photodegradation.

Comparison of nanotechnology based panels and conventional crystalline-based panels in southern Algeria

F. Kaddouri

Faculty of Sciences of M'hamed Bougara University, and the Laboratory of Motor Dynamics and Vibroacoustics of the Faculty of Technology of M'hamed Bougara University of Boumerdes, Algeria

Corresponding author: f.kaddouri@univ-boumerdes.dz

Abstract:

In this paper, the author present a study on a pilot project of a solar plant launched in the city of Ghardaia, Algeria as part of the country renewable energies policy to face global and sustainable environmental challenges such as greenhouse effect and air pollution; which are known to be limited by using renewable energy sources. Two different photovoltaic technologies, nanotechnology based panels made of CIGS and CdTe thin films together with conventional crystalline-based panels,are studied and compared in specific southern Algerian regions characteristics, particularly high temperatures and high temperature gradients. These latter are taken into consideration to study their impact on the energy conversion performance. Finally, recommendations and guiding principles are given to increase the system's output and efficiency.

Theoretical study of the absorbing layer in a CIS solar cell

Bouriche Meriem, Bellal Tahar, Tala Ighil Razika, Toubane Mahdia
ENS-Kouba, Algeria
Corresponding author: meriem.bouriche@g.ens-kouba.dz

Abstract:

Our investigation delves into the CIS absorbing layer, a crucial component of the photovoltaic cell. We commence by defining CIS as a semiconductor primarily composed of copper, indium, and selenium ions. These ions are meticulously arranged in a chalcopyrite-type lattice, adhering to stoichiometric proportions to impart unique properties and distinctive characteristics. We dedicate a portion of this study to unraveling these properties, encompassing optical, electronic, and mechanical aspects. Next, we meticulously examine the layered structure of the photovoltaic cell, meticulously detailing the dimensions of each layer and the materials upon which they are deposited. We delve into the intricacies of the cell's active region, shedding light on its pivotal role in the conversion process. Subsequently, we meticulously analyze the performance characteristics of the photovoltaic cell, encompassing parameters such as Icc, Vco, FF, and η Our exploration extends to the realm of laboratory techniques employed in the fabrication of the CIS absorbing layer. We meticulously evaluate the advantages and disadvantages of each technique, providing a comprehensive overview of the fabrication process. We then turn our attention to the critical factors that influence the energy yield and longevity of the cell, outlining effective storage strategies to maximize its lifespan. Finally, we embark on a comparative analysis, juxtaposing the CIS solar cell against its traditional counterpart, the silicon crystal-based cell.

Impact of diffused elements from the metallic substrate on the CISe absorbent layer performances

Messaid Bachir Eddine[1], Tala Ighil Razika [1,2], Lamri Younes[1], Bensouici Fayçal[1], Toubane Mahdia[1], Bouaouina Boujamaa[1,3]

[1]*Research unit of materials processes and environment, UMBB, Algeria*

[2]*Institute of Electrical & Electronic EngineeringUMBB, Algeria*

[3]*Laboratoire Revêtement, Matériaux & Environnement,UMBB, Algeria*

Corresponding author: b.messaid@univ-boumerdes.dz

Abstract:

This study is interested in the elaboration of the absorbent layer CuInSe2 by a less expensive technique "Spray Pyrolysis", a comparative study was based on the use of two substrates, the glass substrate and the Stainless steel 316 , the XRD of the CISe deposited on glass shows the presence of four peaks, indexed as (112), (220), (400), and (424). We remark than the intensity of peak this peak improve with the increase in temperature, and its diffraction angle 2θ changes towards the preferential position, We note a good Cu/In and Se/Cu ratios, confirming a good stoichiometry of CISe at 550°C, the CISe have good optical absorption, especially in the visible range. However the CISe layer deposited on stainless steel shows a great loss of crystallization especially with the high temperature of 550° C, the chemical ratios show a bad formation of CISe. Furthermore, EDX specters for the two layers CISe shows that, a Na signal is observed in the CISe deposited on glass, however, metallic impurities were observed in the CISe layer deposited on stainless steel.

Keywords: CuInSe2 solar cells, XRD, EDX , glass substrate , Stainless steel 316 , metallic impurities.

Investigation of High Sintering Pressure Effect on Reduction of the Average Diameter of Glass Foam Pores

Nacira Stiti[1], Fayrouz Benhaoua[1], Salem Boudinar[2], Younes Lamri[1]

[1]*UR-MPE, University of Boumerdes, Algeria*

[2]*LPCM, University of Tizi-Ozou, Algeria*
Corresponding author: n.stiti@univ-boumerdes.dz

Abstract
Glass foam is a good quality insulating material due to its great lightness and its very low coefficient of thermal conductivity. The microstructure of glass foam is characterized by very high closed and partially open porosity; the size of these pores is mainly micrometric. This material is generally manufactured using the compact powder melting method (PCM), the principle of which is to press then heat a mixture of powders. The compaction pressure is an important parameter in this method; it strongly contributes to the expansion of the glass and the change in the shape and size of the pores. This paper presents the study of the effect of high compaction pressure on the microstructure of glass foam. Two samples were prepared using the PCM method by applying two compaction pressures of 65 and 70 MPa. The microstructure was analyzed by scanning electron microscopy (SEM) and the results showed that compaction pressure has an effect on both volumetric expansion and average pore diameter. Indeed, the applied compaction pressures led to samples characterized by pores of homogeneous shapes and increasingly reduced sizes creating nanometric pores in the microstructure which improves properties of the material.

Keywords: Glass powder compaction; Compaction pressure; Glass foam; Porosity.

Efficient Electron Transport: Synthesis and Optical Characterization of ZnO Nanoparticles for PSC Applications

Youcef Ayache [1], Mahdia Toubane[1], M'hand Oughanem[2], Nouara Lamrani-Amaouz[2], Ahcen Chaouchi[2],

[1] *UR-MPE, M'hamed Bougara University, Boumerdes, 35000, Algeria*

[24]*LCAGC, UMMTO, 15000, Tizi Ouzou, Algeria.*

Corresponding autor E-mail: y.ayache@univ-boumerdes.dz

Abstract:

The goal of developing effective electron transport layers (ETLs) is essential to increasing the efficiency of perovskite solar cells (PSCs). The fabrication and optical characterisation of Zinc Oxide (ZnO) nanoparticles specifically designed for PSC applications are investigated in this work. A laborious procedure was used to manufacture ZnO nanoparticles, with the focus on optimizing the synthesis conditions in order to achieve improved electron transport capacity. For verification of compatibility with the spectrum response of perovskite materials, the optical properties of the produced nanoparticles, including absorption and emission spectra, were thoroughly analyzed. The findings support the ZnO nanoparticles' ability to function as effective ETLs in PSCs by revealing their advantageous optical properties. The produced nanoparticles have certain optical characteristics that match the perovskite materials' spectrum response, which enhances electron transport in PSC devices. This study reveals ZnO nanoparticles' potential as an affordable and straightforward substitute for electron transport layers in PSCs, with advantageous optical and electrical characteristics. The results support the development of sustainable and cost-effective solar energy solutions by improving renewable energy technology.

Keywords: ZnO; ETL; sol-gel; optical characterization; PSC.

Analysis of a glass foam composite preparedfromwaste for electromagneticwave absorption application

Lamri Younes[1], Benhaoua Fayrouz[2], Messaid Bachir Eddine [1], Stiti Nacira [1], Toubane Mahdia[1],Tala-Ighil Razik[1], Mouhouche Faiza [2],Farouk Mebtouche

[1]*UR-MPE, M'hamed Bougara University, Boumerdes, 35000, Algeria*

[2]*Signals and Systems research laboratory,UMBB, Algeria*

Correspondingauthor : y.lamril@univ-boumerdes.dz

Abstract :

This drives our modern society to material recycling. In this work, absorbers based on glass foam composites have been developed using glass waste (cullet) and metal waste. A combination of cullet, metal waste (between 0% and 20wt.%) and foaming agent (limestone - $CaCO_3$) is milled and transferred to a heat resistant steel mold and heated at the operating temperature (T = 800°C) during 20 min. The resulting foam composites showed a homogeneous structure. The absorption performances of the foams were characterized over the frequency range between 8-12 GHZ (X-band) using a vector network analyzer Rohde & Schwarz type ZNB 20. The results show a variationof the absorption properties (wave attenuation) as a function of the percentage of filler and the density of the foams. The best composite has an attenuation of 0.83 at 9.45 GHz with a density of 0.34 g/cm^3. The reflection results based on these composites are very encouraging. The foam loaded with 12% of the metallic waste shows a weak reflection from -35.97 dB at 11.44 GHZ frequency. The composites elaborated in this work show high performance for the absorption of electromagnetic waves.

Keywords: foam glass, composites, cullet, materials, waste, electromagnetic wave.

Electrochemical deposition of thin film nickel oxide onto macroporous silicon for CO2 gas sensor

K. M'hammedi, M. Berouaken, N. Bourenane, N. Gabouze
Laboratory of Physical-Chemical Inorganics Materials and their Applications, Physics Department, Science Faculty of Blida1 University, 09000 Blida, Algeria
Corresponding author: kawthermhammedi4@gmail.com

Abstract:
Gas sensors based on semiconductor metal oxides (SMOs) composites have been widely applied into environmental monitoring, medical diagnosis, industrial production, and other fields. Nickel oxides (NiO) have been widely investigated due to their potential applications in electrochromic films, optical materials, fuel cell electrodes, sensors, electrochemical capacitors, batteries, etc. Most of these useful functions depend mainly on the composition, configuration and structure. In this work, we report on deposition of Nickel oxides (NiO). NiO was deposited directly on silicon and macroporous silicon (MPS) surface by electrodeposition method. The plating solution consisted of nickel chloride and potassium chloride at a scan rate of 10 mV/s. The gas sensor performances of the NiO/MPS structure were examined at room temperature using a gas sensing system. The deposited films (NiO) were investigated by scanning electron microscopy (SEM) and X-ray diffraction (XRD). SEM images revealed that the films are porous and filled with NiO nanocrystallites. The gas sensing performance for the detection of CO2 at room temperature was investigated. The results indicated a high response of the sensor to CO2, the maximum response was found of 500%. The investigation on response kinetics showed a fast response/recovery time of the sensor.

Effect of Support of Nanooxide CuO-ZnO Catalysts on the Catalytic Hydrogenation Reaction of CO2

Malika Chalal, Djaouida Allam, Smain Hocine
l'université Mouloud MAMMERI de Tizi-Ouzou, Laboratoire de Chimie Appliquée et Génie Chimique (LCAGC),

Abstract:
In this work, several CuO-ZnO supported catalysts, CuO-ZnO /Al2O, CuO-ZnO /SiO2, and CuO-ZnO/MgO were prepared using polyol route and characterized using BET, BJH, XRD, H2-TPR, XPS, and SEM – EDX analytical techniques and subsequently tested in CO2 hydrogenation to methanol. The catalytics results obtained from this study show that the support exerts a significant influence on the activity and selectivity of CuO/ZnO in the hydrogenation of CO2. Over the acidic support, methanol is mainly produced, while the basic support leads to the formation of methane.

Keywords: Polyol method, methanol synthesis, CO_2 hydrogenation, acidic-support.

Developing bio-packaging from marine waste

Mohamed Said Dahmani and Slimane Kadouche
Applied Chemistry and Chemical Engineering Laboratory University of Mouloud Mammeri Tizi-Ouzou
Corresponding author: medsaid.dahmani92@gmail.com

Abstract:
Following the environmental problems orchestrated in recent years due to the production and excessive spread of plastic in various fields, plastic is now a key element in sectors as varied as packaging, construction, transport, health and electronics. Although this material offers many advantages, it also generates negative externalities; in fact, only a small percentage of plastic packaging is collected for recycling and conservation for future use, while the majority is discarded. These negative impacts on the environment mainly concern the degradation of natural systems linked to plastic packaging leaks, particularly in the oceans, and greenhouse gas emissions during plastic production and waste incineration. Is a plastic-free world possible today? Yes, the idea is to manufacture packaging using a resource other than oil, such as biopolymers derived from animal products like chitosan, which is both biodegradable and derived from marine waste.

The main aim of our work is to produce bio-packaging by recovering marine by-products, in particular shrimp waste (shells), by preparing chitosans from chitin purified by basic deacetylation carried out at two different low temperatures (23°C and 20°C) with a low NaOH content (40%) without stirring and for a period of (10 to 35 days). These conditions are completely different from those reported in the literature, i.e. high temperature (100 to 110°C), NaOH concentration of 40 to 60% and a period of several hours with stirring.

Keywords : chitin, chitosan,deacetylation, biopolymers, bio-packaging.

A novel Comparative Study For Simultaneous Determination Of Cd (II) and Pb (II) Based On Ruthenium Modified Screen Printed Graphite Electrode

Kadri Nahla, Chelaghmia Mohamed Lyamine, Ghediri Dalia, Fisli Hassina and Affoune Abed Mohamed

8 mai 1945 university of Guelma

Corresponding author: kadri_nahla@yahoo.com

Abstract:

Environmental pollution caused by toxic heavy metals is a problem harmful to human beings' health. Various analytical methods, such as spectroscopic and electrochemical methods, are used to detect heavy metals. Standard techniques for finding traces of heavy metals include inductively coupled plasma mass spectrometry. Plasma atomic emission spectrometry and atomic absorption spectrometry. In this field, electrochemical methods are the most effective technique for the determination of trace heavy metals.

We offer a novel technique based on three-dimensional (3D) disposable electrochemical sensors with screen-printed graphite electrodes (SPEs) enhanced with ruthenium nanoparticles (RuNPs). This change provides for more efficient and accurate detection of heavy metals especially (Cd2+) and (Pb2+). The electrochemical sensor exhibits excellent performance metrics, including wide linear ranges, low detection limits, selectivity, and stability. Furthermore, it offers practical advantages such as portability and affordability, making it suitable for on-site monitoring applications. In conclusion, this study presents a significant advancement in electrochemical detection techniques, offering a reliable and efficient method for monitoring cadmium and lead contamination in drinking water and environmental samples. This novel sensing platform contributes to the ongoing efforts to safeguard public health and environmental sustainability by providing rapid and accurate analysis capabilities.

Catalytic degradation of dyes by metallic nanoparticles

Asma Bahloul[1] , Samia Bouakkaz[1], Ali Benayahoum[2],
[1]*Laboratory of Applied Chemistry, University of 08 mai 45, Guelma, Algeria*
[2]*Scientific and Technical Research Center for Physical and Chemical Analysis (CRAPC), Algeria*
Corresponding author: basma2765@gmail.com

Abstract:
In this study, we evaluated the catalytic power of Cu/Cu_2O nanoparticles with a 40/60 ratio already synthesized by chemical reduction of $CuSO_4$ with N_2H_4 and tea extract. We used reduction reaction models of 08 azo and non-azo dyes and have selected UV-Visible spectrophotometry to monitor the catalytic reactions. Dye degradation was based on a reduction reaction by $NaBH_4$, and the role of copper nanoparticles is to provide electron diffusion pores (physisorption). The presence of biomolecules on the nanoparticle surface reinforces the interaction between dye molecules and $NaBH_4$. Azo dyes are highly toxic, carcinogenic, mutagenic and poorly biodegradable due to the azo bond and the presence of benzene rings. The total degradation rate is between 42% and 98%, which is due to the size of nanoparticles [8], their enormous specific surface area and their high density of surface functional groups.

Key words: degradation, Dyes, nanoparticles, physisorption.

Reduction of solid waste through the production of glass foam using gypsum and glass waste

Fayrouz Benhaoua[1], Nacira Stiti [1], YounessLamri [1], Djalila Aoufi [2], Abdelouaheb Djeddou [1]

[1]*UR-MPE, M'hamed Bougara University, Boumerdes, 35000, Algeria*

[2]*CRTI- EChahid Mohammed AbassiCheraga, Algiers; Algeria*

Corresponding author: f.benhaoua@univ-boumerdes.dz

Abstract

In this study, we aimed to protect the environment by developing glass foams based on recycled raw materials, specifically gypsum board scraps and waste flat glass after use. These two raw materials were finely crushed and ground to obtain a very fine particle size range. We combined 0%, 5%, and 10% gypsum powder with 1% CaCO3 foaming agent powder, and then completed it with gypsum powder up to 100%. The samples were thermally treated by sintering for 10 minutes at a temperature of 800°C.To evaluate the quality and performance of our materials, we utilized various physicochemical analysis techniques such as XRD, DSC, porosity measurement, mechanical strength characterization, etc. The results obtained demonstrate that our foams exhibit high porosity, exceeding 81%, as well as compression resistance exceeding 05 MPa, These results position our material as a high-quality construction insulation, offering both exceptional performance and a reduced ecological footprint, contributing to a more sustainable future for our planet.

Keywords: Environmental, waste, foam glass, recycling.

Peroxymonosulfate activation by Zinc cobaltite for the Rhodamine B degradation

Sabrina Naama, Soumia Benredouane, Khaled Derkaoui, Afaf Brik, Sihem Bouanik, Seif-Eddine Friha, Toufik Hadjersi

Affiliation of the participant: *CRTSE. 2, Bd. Frantz Fanon, B.P. 140 Alger-7 Merveilles, Alger, Algeria.*

Abstract

The environmental pollution caused by industrial and pharmaceutical waste is now a critical threat to human society. Thus, it is necessary to treat this wastewater in order to preserve the environement. To this end, several methods have been developed to degrade the pollutants, including the catalysis, whichis suitable for the oxidation of a wide range of organic compounds. For that many catalyst have been develppoed such TiO_2, ZnO,…Although zinc cobaltite, a visible light active p-type spinel oxide semiconductor, has been utilized in the oxygen evolution, hydrogen production process, it is scarcely used as catalyst for water depollution. Herein, zinc cobaltite $ZnCo_2O_4$ modified silicon nanowires have been successfully synthesized by a simple hydrothermal method. The silicon nanowires have been elaborated by metal-assisted chemical etching. This design makes it possible to take advantage of both the merits of silicon nanowires and $ZnCo_2O_4$ and their synergistic effect.The obtained samples have been characterized by Scanning electron microscopy with SEM/EDX, XRD, XPS and UV-Vis spectrophotometry. The $ZnCo_2O_4$/SiNWs nanocomposites have been used as catalyst for the rhodamine B degradation by activating peroxymonosulfate (PMS) with different concentrations 5, 25, 35, 50 and 75 micromol/l under ultrasound. The best photocatalytic degradation efficiency of the $ZnCo_2O_4$/SiNWs nanocomposites has been obtained for 35micromol/l of PMS concentration where a degradation 95% has been achieved within 10min.

Effect of Si content on the doping concentration of Al-P+ rear junction for n-PERT Silicon solar cells

Oussama Djema, Abdelghani Boucheham, Abbes Marref, Boutaleb Labdelli , Kheira Bekhedda, Abdelkader Djelloul, Lyes Benharrat 1, Seif-Eddin Friha

Affiliation of the participant: Research Centre in Semiconductors Technology for Energetics (CRTSE), Algiers, Algeria

Corresponding author: djemaoussama@crtse.dz

Abstract:

Due to its outstanding properties, considerable research interest has been drawn to the n-type PERT solar cells. This work aims to investigate the effect of Si content on the doping concentration of Al-P+ rear junction for n-PERT Silicon solar cells. For this, the Al paste was modified by adding Si powder with content up to 3%wt. After that, the prepared Al-Si pastes were screen- printed on the n-type Si wafers. The as screen-printed wafers were then dried at a temperature of 200°C for 5 min and fired in RTP furnace at a set peak temperature of 783 °C under N2 atmosphere to form the AlSi local rear contacts. Electrochemical capacitance-voltage profiler (ECV) showed that the addition of the Si content to the Al paste lead to higher doping concentration. This fact was confirmed by the Scanning Electronic Microscopy (SEM) analysis, showing that the addition of the Si content to the Al paste lead to a thicker Al-P+ rear junction formation.

Keywords: Al paste, Si content, screen printing, n-PERT, Si solar cell.

The influence of the SiO2 oxide in the diffusion mechanism of phosphorus in n-type monocrystalline silicon

B. Labdelli , A. Boucheham, L. Benharrat, A; Djelloul, K. Bekhedda, O. Djema , A. Maref, C. Nasraoui , H. Mazari, A.Bennabi And F. Rahmani

Affiliation of the participant: CRTSE, Alger-, Algeria;

Corresponding author: labdelliB@crtse.dz

Abstract

N-type silicon solar cells have many advantages over p-type cells; they are not subject to lightinduced degradation due to the division of boron-oxygen complexes and they are less sensitive to chemical impurities activated during the diffusion and oxidation steps at high temperatures and they are less sensitive to laser-induced damage. POCl3 diffusion is currently the standard method for the industrial manufacture of n-type emitters. In this work, preform sources are used as dopants (sheets Of Paper Doped with Phosphorus). After the pre-deposition of phosphorus, a glass phosphosilicate (PSG) was removed by soaking in 10% HF. The mechanism of silicon oxidation has been widely examined for half a century due to its importance in the technology of semiconductor devices. Thermal oxidation is a well-known method for passivating the surfaces of c-Si wafers for various applications in microelectronics because thermal silicon oxide offers excellent surface passivation due to its low density of interface defects. In this study, we present the impact of the addition of a SiO2 oxide layer before the construction of the transmitter. To reduce the dead zone, an oxidation step before diffusion is used. The formation of thermal oxide on the surface of the silicon before diffusion can indeed reduce the size of this zone, the SiOx zone, acting as a diffusion barrier to phosphorus.

Effect of viscosity formulation on entropy generation analysis for laminar forced convection flow of AL_2O_3/water nanofluids in a pipe

Leila Saoudi , Mourad Gareche, Nadjet Azril, Noreddine Zeraibi
Affiliation of the participant: Laboratory of Engineering Physics hydrocarbons,UniversityM'hamedBougaraBoumerdes, 35000, Boumerdes, Algeria
Corresponding author: E-mail:l.saoudi@univ-boumerdes.dz

Abstract:
Laminar regime was assumed, in the analysis of the flow of Al_2O_3-water nanofluid flowing through a horizontal copper tube under constant temperature boundary conditions at the wall. This study was performed with three viscosity models available in the literature, based on the analysis of entropy generation. The effects of nanofluids concentration ϕ(0%–4%), Reynolds number Re (200–2200), nanoparticles diameters dp (10 and 40nm) and inlet temperature (25°C and 50°C) on the evaluation of thermal and frictional entropy generations are discussed.

Key words: Circular tube; Entropy generation; Laminar flow; Nanofluid.

Characterization of asphaltenes from Hassi-Messaoud oil by NMR

Khadidja Kradra Brahma[1,2], *Souad Bennabi*[2,3], Amina Sardi[1,2,3] and Soumia Abdelkrim[4]

[1]*LCPM,Faculté des Sciences, Université d'Oran1, Algérie,*

[2]*LCMCR, Hassiba Benbouali Université de Chlef, Algerie.*

[3]*Département de Chimie, UHBC, Chlef, Algérie.*

[4]*Laboratoire de Chimie des Matériaux, Université d'Oran1, Algérie*

Corresponding author: k.brahma@univ-chlef.dz

Abstract :

Crude oil is a complex mixture of hydrocarbons and heteroatomic compounds of different polarities and molecular weights. One possible classification of petroleum compounds consists of separating a crude oil into four chemically distinct fractions: saturates, aromatics, resins and asphaltenes. Asphaltenes are defined as the polar, non-volatile fraction of crude oil that is insoluble in light n-alkanes, such as n-pentane or n-heptane and are soluble in toluene. This definition implies that asphaltenes contain different molecular structures. All asphaltene molecules are composed of groups having aromatic polycyclic rings surrounded by aliphatic chains. Asphaltenes aggregate easily, forming aggregates whose stability in the petroleum environment depends on numerous factors. The main objective of this work is to determine the structural parameters of asphaltenes extracted from a deposit of an oil well in Hassi Messaoud to lead to the proposal of representative chemical structures. To do this, different physicochemical and spectroscopic characterization techniques are used. Thus, nuclear magnetic resonance will be used for the structural investigation of molecules.^{1}H NMR and ^{13}C NMR Fourier transform spectroscopies combined with elemental analysis lead to the determination of aromaticity, in agreement with direct data from the ^{1}H NMR spectrum, and of the average number of carbon atoms per aliphatic chain.

Removal of Evans Blue Dye of Wastewater using Metal-Organic Framework (MOF) mixed with Layered Double Hydroxide (LDH)

Bennabi Souad[1,2], *Kradra Brahma Khadidja*[2,3,4], *Sardi Amina*[1,2,3]

[1]*Department of Chemistry, University of Chlef, Algeria*

[2]*LMCCR, Faculty of Exact Sciences and Informatics, University of Chlef, Algeria*

[3] *L.C.P.M, University of Oran1, Algeria.*

[4]*Département des sciences de la nature et de la vie, UHBC, Chlef, Algérie.*

Corresponding author : s.bennabi@univ-chlef.dz

Abstract

The latest research efforts have focused on creating innovative and exceptionally effective adsorbents that can overcome the constraints of conventional methods for wastewater treatment. Within this context, two materials: Metal-Organic Frameworks (MOFs) and Lamellar Double Hydroxides (LDH) gain the attention of the scientists. In this work, we report the synthesis of a new hybrid material based on MOF-ZnPA (MOF: Metal Organic Framework, Zn: Zinc, PA: Pyromellitic Acid) and Co-Zn-Al-Co_3 Layered Double Hydroxide (LDH) via a facile solvothermal method using DMF (N,N'-Dimethylformamide) as solvent. The structure and morphology of the synthesized new material have been investigated by X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) which confirmed obtaining MOF-ZnPA/LDH at different percentages of LDH (10, 30, and 50%). The adsorption characteristics of the synthesized materials for the Evans Blue dye showed an adsorption capacity of 246 mg/g for MOF-ZnPA/LDH compared to 141 mg/g for MOF-ZnPA without LDH after 40 minutes of contact time.

Development and characterisation of an acetonevapour detector based on a functionalisedkeratin/(x%)-carbon fibre biocomposite

Rachida Douani, Hayet Hammouche, Malika Saidi, M'hand Oughanem, Ahcene Chaouchi

Affiliation of the participant: LCGC, Mouloud Mammeri University of Tizi-Ouzou.

Corresponding author: rachida.douani@ummto.dz

Abstract :

This research consisted of developing acetone vapour sensors based on a keratin/x% FCF biocomposite. The keratin was extracted froms heep woolusing a mildalkaline treatment. The carbon fibres were functionalized using a strong acid treatment. The resulting materials were analysed by SEM, FTIR and UV-visible. The performance of our sensors wase valuated by measuring the impedance (Z) at a frequency of 1 KHz at different temperatures and concentrations of acetone gas.

The results of the structural and morphological analyses confirmed the structure of the keratin gel and the presence of oxygen functional groups on the surface of the carbon fibres. Impedance measurements showed that the incorporation of the functionalized carbon fibres into the keratin matrix reduced the operating temperature of the sensor from 125°C for the pure keratin-based sensor to 110°C for the biocomposite-basedsensor. There was also a significant improvement in the sensitivity of the sensor, which increased from around 6.45 to 2985%. It is there fore concludedthatkeratin/FCF biocomposites are promising candidates for acetonegasdetection.

Keywords: carbon fibres, functionalised, keratin, gas detector, acetone, operating temperature, sensitivity.

Advancements in Nanomaterials for Photon Detection: Applications in Silicon Photomultipliers

Faiza Hadji, Ali Benouadah , Bouzid Boussaha
University of Algiers 1, Benyoucef Benkhedda. Laboratory of Materials Sciences and Environment SDME
Corresponding author: f.hadji@univ-alger.dz

Abstract :
SiPMs, with micrometric channels and millimetric pixels, have found extensive use across diverse fields like medicine, high-energy physics, spectroscopy, biology, and LIDAR. Their integration into large-scale devices underscores the prowess of silicon technology in enhancing sensitivity and versatility in detecting photons. In a comparative study evaluating SiPM models, including the Hamamatsu S13360-6075PE, SensL MicroFJ-60035-TSV (J-series), and KETEK PM3325-WB-D0, it was observed that these sensors exhibit varying Photon Detection Efficiency values, with peaks around 420nm ranging from 40% to 50%. Among these models, the SensL MicroFJ-60035-TSV (J-series) SiPM demonstrated superior overall performance, boasting higher PDE values across the spectrum. The findings highlight the significance of careful sensor selection in optimizing photon detection capabilities. The SensL MicroFJ-60035-TSV (J-series) SiPM, with its enhanced PDE values and compact design, emerges as the preferred choice for applications requiring precise and efficient photon detection.

Keywords: SiPM, Performances, Photons, detection, nano-technology.

Elaboration des capteurs piézoélectriques à base de kératine pour la récupération d'énergie

Hayat Hammouche , Saliha Rabhi , Rachida Diouani
Laboratoire de chimie appliqué et Génie chimique (LCAGC), Algeria
Corresponding author: hayat.hammouche@ummto.dz

Abstract :

La kératine est un biopolymère offre l'avantage d'être largement disponible dans la nature, ce qui en fait un matériau durable et respectueux de l'environnement pour une variété d'applications biotechnologiques et biomédicales. En raison de sa structure moléculaire asymétrique, la kératine est capable de générer une charge électrique en réponse à une contrainte mécanique, et vice versa. Cette étude est consacrée à l'élaboration des capteurs flexibles à base de kératine2 wt% Gly et kératine/ 2 wt % Gly / 0.2 % fibre de carbone. Les films ainssi élaborés ont été caractérisés par différentes techniques d'analyse (MEB, FTIR....). Les caractérisations par impédancemètre a montré que le film kératine/ 2wt% Gly /0.2% fibre de carbone présente de propriétés diélectriques meilleurs que le film de kératine flexible pur. Les deux types de capteurs ont pu générer une tension de sortie après l'application d'une force sous la pression du doigt. Des tensions de 10.4 Volte et 2.4 Volt ont été enregistré respectivement par le composite et kératine/ 2 wt% Gly / 0.2 % fibre de carbone. Ces résultats montrent que ces films peuvent constituer un choix prometteur l'alimentation des dispositifs électronique portable et implantable à faible consommation.

A Sustainable Approach for Medical Applications of Green Synthesis of Nanoparticles from Algerian Plant Extracts

Bakdi Hadjer, Salima Kebbouche-Gana And Djelalli
Laboratoire de Genie de la reaction, USTHB
Corresponding author: hadjer.bakdi@usthb.edu.dz

Abstract:
In this study, we present a novel method for the biological synthesis of silver nanoparticles (AgNPS) utilizing hot water extracts from indigenous plants as a reducing agent. Our protocol outlines a green synthesis route that has demonstrated remarkable antibacterial properties, employing leaf extracts sourced from medicinal plants.
To characterize the synthesized AgNPs comprehensively, we employed advanced analytical techniques including UV–Vis spectroscopy, Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). The UV–Vis spectroscopic analysis revealed a surface plasmon resonance of AgNPs at approximately 445 nm, indicative of their unique optical properties. Furthermore, FTIR spectroscopy unveiled the presence of distinct functional groups within the nanoparticles. Our investigation also determined the average crystallite size of AgNPs to be 25.52 nm, underscoring their nanoscale dimensions ideal for various biomedical applications. Additionally, SEM imaging confirmed the spherical morphology of the synthesized AgNPs, further validating their suitability for medical purposes. In summary, our study highlights the potential of green synthesis methodologies using natural plant extracts for the production of silver nanoparticles with promising biomedical attributes, paving the way for sustainable and environmentally conscious nanomaterial synthesis practices.

Green synthesis of zinc oxide nanoparticles and evaluation of their properties

Kheira Haiouani[1], *Ziane Achour*[2]

[1] *Department of Chemistry, Laboratory of Organic Chemistry and Natural Substances, Faculty of Exact Sciences and Informatics,*

[2]*University of Djelfa, Algeria*

Corresponding author: kirahaiouani@yahoo.fr

Abstract:

Zinc oxide nanoparticles (ZnO NPs) were prepared using clove oil. GC-MS analysis demonstrated that Eugenol is the main bioactive compound of the prepared extract. Experiments were designed, based on the central composite design. The effects of different amounts of zinc chloride and clove oil were evaluated for antioxidant and bactericidal properties of the formed ZnO NPs using the response surface methodology. The attained results demonstrated that more desirable NPs with maximum antioxidant activity and bactericidal effect, against Escherichia coli and Staphylococcus aureus. Furthermore, XRD and SEM analysis results revealed that the fabricated ZnO NPs had a hexagonal shape and could degrade methylene blue during UV radiation.

Keywords: antioxidant activity, clove oil, hydrodistillation, photocatalytic activity, zinc oxide nanoparticles.

α-TOCOPHEROL attenuates the oxidative stress induced by the anticancer " CARBOPLATIN " on sperm cells

Nourelhouda Benamara, Lamine Bournine, Sihem Bensalem, Mokrane Iguer-Ouada.

Bedjaia university

Corresponding author: nourelhouda.benamara@univ-bejaia.dz

Abstract:

This study aims to explore the direct consequences of Carboplatin (CBDCA) on mature spermatozoa and assess the protective capabilities of an antioxidant, namely vitamin E, against the toxicity induced by this anticancer agent. Both the direct exposure of spermatozoa to CBDCA and their co-incubation with vitamin E were scrutinized utilizing computer-assisted sperm analysis (CASA) to evaluate sperm mobility parameters. The underlying molecular mechanism driving this toxicity was determined by examining the levels of malondialdehyde (MDA), a byproduct of lipid peroxidation.

The findings reveal that CBDCA adversely affects spermatozoa mobility, as evidenced by decreased values of VSL (5.51 ± 0.64 µm/s) and PR (2.80%) compared to the negative control (10.97 ± 0.42 µm/s and PR of 17.23%), with the effects becoming particularly pronounced after 60 minutes of co-incubation. This effect is attributed to the induction of lipid peroxidation in the sperm membrane, leading to elevated MDA levels (4.498 ± 1.18) compared to the negative control (0.864 ± 0.59). Furthermore, vitamin E demonstrates a potential protective effect against CBDCA toxicity, as evidenced by increased values of VSL (7.67 ± 0.42 µm/s) and PR (8.99%). Consequently, CBDCA impacts spermatozoa mobility by exacerbating oxidative stress, resulting in elevated MDA levels. However, the detrimental effect is mitigated following treatment with vitamin E (2.46 ± 0.93).

Comparative phytochemical analysis of a medicinal plant from two distinct geographical areas

Zerrouk Roumeila, Boudermine Sihem, Charif Guiassa
Faculté des sciences, département de chimie, université 20 Août 1955-skikda
Corresponding author: r.zerrouk@univ-skikda.dz

Abstract:
Apiaceae is a family of mostly aromatic flowring plants. This work concerns the biological evaluation of a species of the apiaceae family between two regions, Algeria and France. After extraction of the aerial parts of the plant; tests were carried out on the different biological activities of its extracts in solvents of increasing polarity. The antioxidant activity shows that the Algerian flora is much stronger than that of the French plant. Phytochemical investigation of the plant explains the difference between the two regions. Crop quality and the climatic difference between cold and humid.

Keywords: medicinal plant, apiaceae family, extract, antioxidant activity, plant, biological.

Sustainable Synthesis of High-Quality Zinc Oxide Nanoparticles Using Nonthermal Plasma

Bounedjar Nourelhouda, Ferhat Mohammed Fouad, Toukal Linda, Messai Ridha, Allag Nassiba, Humayun Muhammad, Ficai Anton, Hamoudi Said Ammar, Bououdina Mohamed*
UDERZA, University of El Oued, Algeria
Corresponding author: nourelhouda-bounedjar@univ-eloued.dz

Abstract:
This study presents a sustainable synthesis method for zinc oxide (ZnO) nanoparticles using nonthermal plasma, employing water as the sole solvent and a zinc precursor as the primary product, with humid air serving as the gas vector. This eco-friendly approach aims to minimize environmental impact by eliminating the need for organic solvents and reducing energy consumption. The synthesized ZnO nanoparticles exhibit high crystallinity and purity, with a consistent rod-like shape and minimal contamination, as confirmed by TEM and EDS analyses. The hexagonal wurtzite structure of ZnO nanoparticles, characterized by lattice constants a = 3.25 Å and c = 5.21 Å with a c/a ratio of 1.60, was confirmed through XRD and Rietveld refinement analysis, indicating high phase purity, minimal lattice distortion, and a uniform crystallite size of approximately 63.09 nm, with calculated stress at -0.1371 GPa suggesting expansion, making them suitable for applications in electronics, photonics, and corrosion inhibition. X-ray photoelectron spectroscopy (XPS) analysis confirms zinc predominantly in the Zn^{2+} oxidation state and oxygen in the form of oxide O^{2-}, verifying the success of the synthesis process. These results demonstrate the efficacy of nonthermal plasma synthesis in producing high-quality ZnO nanoparticles, highlighting its potential as a green and sustainable method for nanoparticle fabrication.

Keywords: Sustaible, Zinc oxide nanoparticles, X-ray photoelectron spectroscopy, eco-friendly.

Nanoparticles in Food: A Promising Vision for Food Innovation, Safety, and Sustainability

Yahiaoui Karima[1], Lefkir Samia[1], Laoufi Razika [2], Youyou Soraya[1], Hamdis Nacim[1]

[1]Laboratory of food Technology, University of Boumerdes, Algeria.

[2]Laboratoire de technologie douce et valorisation des matériaux biologiques et biodiversité Boumerdes, Algeria.

Corresponding author: k.yahiaoui@univ-boumerdes.dz

Abstract

In the near future, the use of nanoparticles in food offers promising potential to enhance the quality, safety, and shelf-life of food products. By harnessing the unique properties of nanoparticles, we can develop new approaches to address current challenges in the food industry. The first opportunity lies in using nanoparticles as functional food additives. These nanoparticles can improve the properties of food products, such as texture, stability, and controlled release of active ingredients. This paves the way for healthier, functional, and personalized foods that can meet the specific needs of consumers. Furthermore, nanoparticles can be incorporated into food packaging materials to enhance their barrier properties against gases, moisture, and contaminants. This can extend the shelf-life of food, reduce food waste, and improve product safety. Another promising aspect is the enhancement of nutrient bioavailability through nanoparticles. By encapsulating nutrients within nanoparticles, we can increase their absorption and utilization by the body, thereby contributing to better nutrition and improved health. Lastly, nanoparticles can also play a key role in the detection and prevention of food contaminants. Their use as probes and sensors enables rapid and sensitive detection of pathogenic bacteria, pesticide residues, and other undesirable substances, ensuring food safety.

Nanoparticles in the Food Industry: Risks, Hazards, and Regulations

Yahiaoui Karima[1], Lefkir Samia[1], Laoufi Razika [2], Youyou Soraya[1], Hamdis Lahcen[1]

[1]Laboratory of food Technology, University of Boumerdes, Algeria.

[2]Laboratoire de technologie douce et valorisation des matériaux biologiques et biodiversité Boumerdes, Algeria.

Corresponding author: k.yahiaoui@univ-boumerdes.dz

Abstract:

This summary examines the applications of nanoparticles in the food industry, associated risks, and the existing regulations in place to safeguard consumers. Nanoparticles are utilized in various food applications, such as additives, packaging, and improving food quality. However, it is crucial to understand the potential risks they may pose to human health. Their small size grants them unique properties but also raises concerns regarding their toxicity and ability to cross biological barriers. To ensure consumer safety, strict regulations have been implemented. These regulations require comprehensive risk assessments prior to the use of nanoparticles in the food industry. Studies are conducted to evaluate their stability, bioavailability, potential tissue accumulation, and impact on human health. These safety assessments are crucial for making informed decisions regarding the use of nanoparticles. Regulations pertaining to nanoparticles in the food industry vary across countries and regions, but they all aim to minimize potential risks for consumers. Concentration limits, labeling requirements, and good manufacturing practices are often enforced to ensure the safety of food products containing nanoparticles. It is important to emphasize that continuous research and monitoring are necessary to assess long-term risks and adapt regulations accordingly.

Nanotoxicity of TIO2-NPs induced ROS generation on Wistar Rats

Bouzenzana Sara, Rouabhi Rachid, Bouzenzana Abdellali
Tebessa university
Corresponding author: sara.bouzenzana@univ-tebessa.dz

Abstract:
TiO2 nanoparticles (nano-TiO2) are one of the most widely used nanomaterials in many sectors such as cosmetics, food, medicine, solar energy conversion, catalysis, agriculture, and water purification.
Moreover, The great demand and widespread applications of TiO2-NPs will inevitably cause damage to organisms and ecosystems. because the size of nanoparticles is similar to that of typical cellular components and proteins, nanoparticles can travel inside the human body and induce the production of ROS causing adverse biological consequences, which include the generation of superoxide anion (O·−2), hydrogen peroxide (H2O2), and hydroxyl radicals (·OH), this would result in cell death due to oxidative DNA damage and many other diseases. The purpose of this study was to systematically research the influence of nanotoxicity of TiO2-NPs on Wistar rats after an oral administration for 90 days at the renal level. The experiment was conducted on 21 Wistar rats (males). The results were determined with the variation of MDA, and GPX activity treated with TiO2 NPs compared to the controls, in our work we observe that there is a highly significant increase in the batch treated with TiO2 NPs at a dose (2.5 ml/kg/day).

Key words: TiO2-NPs, ROS, Wistar rats.

Employing Biological Nanovectors for Food Preservation

Yahia Bellil[1,2], *Wassila Chahrour Bellil*[1,2], *Taha Ahmed Benabbou*[1], *Zineb Benmechernene*[2], *Mebrouk Kihal*[2]

[1]*LBPBVP, University of Saida,, Algeria*
[2] *LMA, University of Oran 1, Algeria.*
Corresponding author: *yahia_bellil@yahoo.fr*

Abstract:

Nanotechnologies offer exciting prospects for food safety. The use of nanoparticles in food items is still limited despite their ability to penetrate packaging, particularly in agriculture and the food industry. As such, there is an ongoing pursuit of new technologies to enhance food preservation, taste, flavor, and texture. In this study, sixteen lactic acid bacteria strains previously isolated from fermented products were selected to assess their probiotic potential and their ability to control the growth of a pathogen in a model food matrix (fresh beef meat) after encapsulation in starch-based nanoparticles. The results show that three strains, identified as potential probiotic candidates, encapsulated in nanoparticles, were able to control the growth of the pathogen bacteria Listeria ivanovii in the meat after fourteen days of storage at 4°C. Nanoparticles can be chemically more reactive and more bioactive than larger particles, but their use may increase agriculture's reliance on chemical-based techniques and high energy consumption. It is crucial to minimize the distance between consumers and producers to address these concerns.

Keywords: lactic acid bacteria, preservation, food, Nanotechnologies, Nanoparticles, beef meat.

Strategy of screening and optimization of process parameters using experimental design: Application Optimization of graphene production

Soumia Benredouane, Sabrina Naama , Amal Elfiad, Madjid Ifires,Toufik Hadjersi
CRTSE, Algeries, Alegria
Corresponding author: benredouane_s@hotmail.fr

Abstract :
In recent years, statistical methods have seen widespread application in the design of experiments across various scientific domains. The design of experiments serves as a valuable tool, providing statistical models that aid in understanding the interactions between optimized parameters. Additionally, response surface methodology (RSM) has emerged as an effective tool for constructing quadratic regression models, thereby quantifying the relationship between controllable input parameters and the resulting response surfaces.
The primary objective of this study is to identify the optimal conditions for synthesizing graphene through the electrochemical exfoliation method, employing response surface methodology.

Keywords: Graphene; Graphite rods; Optimization; Central composite design;Electrochemical exfoliation

Enhancing Behçet's Disease Management through Nanotechnology: Insights and Future Directions

Messaoudene Djamel [1] , *Ghozali Nourelhouda* [1,2]

[1:] *Laboratory of Biodiversity, Biotechnology, Environment and sustainable Development, FS,UMBB.*

[2:] *Team "Cytokines and NO synthases: Immunity and pathogenesis", LBCM, FSB, USTHB, Algiers, Algeria.*

Behçet's disease (BD) is a chronic, multi-systemic inflammatory disorder characterized by recurrent oral and genital ulcers, uveitis, and a variety of systemic manifestations. Conventional treatment options, including corticosteroids and immunosuppressants, often lead to significant side effects and may not be effective for all patients. Recent advances in nanotechnology have opened new avenues for the treatment of BD, particularly through the use of nanoparticles (NPs). Nanoparticles offer unique properties such as enhanced bioavailability, targeted drug delivery, and controlled release profiles, making them promising candidates for improving BD management. This study explores the potential of nanoparticles including liposomes, polymeric nanoparticles, and metallic nanoparticles, in the treatment of BD, to deliver drugs more precisely to affected tissues, reducing overall systemic exposure and associated side effects. We will discuss ongoing research into nanoparticles encapsulating specific drugs or anti-inflammatory agents, targeting pathways involved in the disease process. The integration of nanotechnology in BD treatment holds promise for reducing systemic side effects, improving patient compliance, and ultimately enhancing therapeutic outcomes. Further clinical studies are required to validate the efficacy and safety of nanoparticle-based therapies in BD patients.

Key words: Behçet's disease, nanoparticles, inflammation, immunomodulation.

Entropy generation of ferrofluid under a magnetic field

Abdelaziz Boumaiza, Cherif Ould Lahoucine, Mahfoud Kadja
Laboratory of Applied Mechanics of New Materials - LMANM, Department of Mechanical Engineering, Faculty of Sciences Technology, University of May 8, 1945 Guelma, Algeria.
Corresponding author: azize2520@gmail.com

Abstact:
In this work, three-dimensional numerical simulation is used to examine the effects of a uniform external magnetic field on entropy generation of ferrofluid flow in a wavy channel. The non-wavy portion of the channel is thermally insulating, but the wavy surfaces at the top and bottom of the channel are heated with a uniform heat flux. A regular magnetic field is applied along the direction of the main flow in the wavy part, in a direction perpendicular to the flow. The study investigates the effects of magnetic field strength, Reynolds number, and volume fraction on entropy generation .The results indicate that the magnetic field has a greater effect on entropy generation at low Reynolds numbers (less than 400). The minimum entropy generation is obtained at Re = 1200, B= 300, and ϕ = 2%.

Localized surface magnon modes in bcc ferromagnetic lattices

Rebiha Challali, Boualem Bourahla, Smail Sait
UMMTO- Tizi-Ouzou
Corresponding author: rebiha.challali@ummto.dz

Abstact:
The physical, chemical and magnetic properties of materials change significantly by moving from the perfect zone called bulk to the surface region. The presence of surface destroys the periodicity of a crystal, and leads to additional precession modes not present for the bulk. They are distinguished in two categories: (a) Surface localized spin modes, whose frequencies are external to the bulk spectrum and (b) Scattering spin waves, which penetrate deeply the bulk and added to the bulk modes.
Spin dynamics, magnon scattering and surface localized spin states in cubic ferromagnetic systems are the subject of our study (the case of body cubic centred lattice). Based on the function method of Green, we consider the surface as a perturbation at the semi-infinite crystal.
The localized magnon spectrum derived from the elements of a Landauer-type scattering matrix. The magnon properties are simulated and are determined numerically using the matching method. The normalized energy of spin waves is analysed as a function of the exchange integral parameters, from softening to hardening in the boundary of the surface region. The observed fluctuations in the numerical results demonstrate the interference magnon effects between scattered spin waves and the localized magnon states, generated by the surface region with characteristic Fano resonances.

Keywords: Spin waves; Localized spin states; Ferromagnetic cubic lattices; Fano resonance.

Docking study to treat the Omicron variant of COVID-19 infection using biosynthesized ZnO@Fe3O4 nanocomposites

Meneceur Souhaila, Salmi Chaima, Laouini Salah Eddine, Hamdi Ali Mohammed, Khezzane Anouar

University of El Oued

Corresponding author: menaceursouheila@yahoo.fr

Abstact:

The global health crisis brought about by the SARS-CoV-2-induced COVID-19 pandemic has underscored the need for immediate endeavors to identify effective treatments. Molecular docking has emerged as a valuable resource in the field of drug discovery, enabling the investigation of potential interactions between small molecules and target proteins.in this study, molecular docking studies were conducted to upgrade Fe3O4 nanoparticles to ZnO@Fe3O4 NC to enhance composite efficiency. Leveraging the FDA-approved use of Fe3O4 nanoparticles and their known antiviral activity, our docking experiment demonstrated promising results in the interaction between ZnO@Fe3O4 nanocomposite and the spike protein receptor-binding domain of SARS-CoV-2 S Omicron. These findings suggest that ZnO@Fe3O4 nanocomposite could potentially inhibit virus attachment to host cell receptors more stably, providing a promising avenue for further exploration in developing effective medications against SARS-CoV-2.

First-principles calculations of the structural, electronic properties of quaternary semiconductor chalcopyrite

Sassoui khadidja
Department of Physics, Faculty of Science, University of M'sila, Algeria.
Corresponding author: sassouikhadidja96@gmail.com

Abstact:
The interest in chalcopyrite material semiconductors has increased due to their potential uses in various fields such as light-emitting diodes, nonlinear optics, photovoltaic systems, solar cells, and high-temperature thermoelectric applications. This research explores the structural and electronic properties of BeSiP2xSb2(1-x) quaternary alloys. These alloys are variations of chalcopyrite semiconductors and are studied for different compositions (x=0, 0.25, 0.5, 0.75, and x=1). We used the plane wave pseudo-potential approach within the density functional theory (DFT) framework and applied the generalized gradient approximation (GGA). The findings suggest that substituting Sb for P in the alloys leads to a reduction in the unit cell volume and an increase in the energy band gap, with values ranging from 0.519 eV to 1.194 eV.

Keywords: Chalcopyrite materials semiconductors, DFT, quaternary alloys, pseudo-potential approach.

Spin waves dispersion in periodic multilayers: Application to Fe/Dy

Haddag Ouiza, Ouahiba Nafa, Boualem Bourahla
Laboratoire de physique et chimie quantique -Université Mouloud Mammeri de Tizi-Ouzou
Corresponding author: ouiza.haddag@ummto.dz

Abstact:
In this present work, we investigated the dynamics of spins in Transition Metals/Rare Earth (MT/TR) multilayers. Currently the type of systems has been the subject of numerous studies due to their interesting characteristics. The choice of the Fe/Dy multilayer system is linked, particularly, to its extraordinary properties. Specifically, the exchange interactions due to Dy give them a Curie temperature higher than ambient temperature, thus allowing these multilayers to be magnetized at ambient temperature. Additionally, they exhibit a high coercive field, significant Kerr rotation, as well as a strong magnetization. For the study, we used the Heisenberg model because it well describes the quantum spin exchange interactions in a ferromagnetic crystal lattice. The Hamiltonian makes it possible to write the equations of motion for spin precession in infinite ferromagnetic multilayers made up of n atomic planes of iron and n atomic planes of dysprosium. The systems studied are made up of pure planes of each species of Fe or Dy atoms. We considered three cases of ferromagnetic multilayers, characterized by the number of atomic planes n (n = 3, 5 and 7) of Fe and Dy. The results obtained show, for the three cases examined, the presence of a single acoustic mode, which corresponds to the phase precession of neighboring sites, and 2n-1 optical modes, which are in phase opposition. These magnon modes essentially depend on n. We conclude that the thickness is an important parameter in the dispersion of magnons.

Vibrational properties of bcc nanojunctions: Application to the interface Iron-Cobalt

Smail Sait and Boualem Bourahla
Faculty of Science, M. Mammeri University
Corresponding author: smail.sait@ummto.dz

Abstact:
The motivation for this work is to introduce a model for an atomic interface, whereby its mechanical properties can be analyzed via its vibration spectra. The model system consists of two semi-infinite body centered cubic crystals joined by an atomic interface A/B, in the direction (100). It is applied to the Fe/Co nanojunction and its inverse Co/Fe.
We calculate the vibration spectra and the phononic conductance, in the harmonic approximation, for the irreducible set of sites that constitute the interface zone. The nanojunction observables are numerically calculated for two cases of elastic hardening and softening, to investigate how the local dynamics can respond to changes in the microscopic environment on the interface domain.
The theoretical calculations of the vibration properties are carried out using the matching method. The possible experimental measurements of this ballistic transmission in comparison with theoretical results should be a useful probe for the determination of alloying force constants across the interface between two such elements. The analysis of the vibration spectra identifies characteristic features and demonstrates the central role of a core subset of sites in the interface domain.

First-Principle Computed Structural and Electronic Properties of CuAlS2

Bekhedda Kheira, Sabiha Anas, Abdallah Trad Khodja, Yacine Fouad Ghrici , Noaman Boukhari

USTO-MB-Oran

Corresponding author: kheira.bekhedda@univ-usto.dz

Abstact:

To investigate structural and electronic of chalcopyrite from the I-III-VI2 family. The calculations are conducted using full-potential linear-augmented-plane-wave (FP-LAPW) method within the revised generalized gradient approximation of Perdew–Burke–Ernzerhof (GGAPBEsol). Learn more about CuAlSe2, which is particularly interesting in scientific communication due to its properties.

Our calculations show a good agreement between our estimated structural properties, such as the maille parameters (a, c, c/a, and), the bulk modulus B and its derivative B', and experimental and theoretical results from the literature. Furthermore, these results show that CuAlS2 compounds have semiconductor behavior with an direct gap. Our charge density calculation using the dense plan (110) revealed that our compound is governed by iono-covalent electronic connections.

Keywords: ab-initio, FP-LAPW, GGA, CuAlSe, direct gap.

Predicting adsorption-induced frequency shift in Functionally Graded Porous nanobeam-based microsensor including Small-Scale Effect

Khouni Soumia, Hicham Bourouina, Abir Lamari, Mohamed Mektout, Yahia Maiza.

Higher Normal School of Bou-saada, Algeria

Corresponding author: khouni.soumia@ens-boussada.dz

Abstact:

This study probes the intricate dynamics of functionally graded porous nanobeam systems, shedding light on the adsorption-induced frequency shifts of a functionally graded porous nanobeam-based microsensor system governed by non-local elasticity theory, which is critical for developing mass detection technologies. The nanobeam structure, characterized by evenly dispersed porosity, is modeled using the elasticity theory of Eringen to capture small-scale behavior. The study presents dynamic equations incorporating explicit shear force and bending moment for both the Levinson beam model (LBM) and Euler beam model (EBM) frameworks, offering a holistic understanding of the nanobeam's response. The research explores the influence of porosity on the structural dynamics and adsorption phenomena. Adatom interactions are meticulously modeled using van der Waals (vdW) forces, incorporating adatom-adatom and adatom-substrate energy contributions within the Lennard-Jones (6–12) potential. The proposed approach is applied to the H/Au(100) system, revealing that the observed frequency shift is contingent upon factors such as porosity, power-law index, small-scale, and adsorption density.

Keywords: Adsorbed adatoms, Nonlocal elasticity, van der Waals Interactions, Porosity, Small-scale effect.

Buffer layer thickness and temperature effects on p-CZTS/n-Zn(S,O)/ITO solar cells

Amria Bencherif, Essaid Bousbiat, Assia Bouraiou and Fatiha Daoudi
Department of Physics, UMBB, Algeria.
Corresponding author: a.bencherif@univ-boumerdes.dz

Abstact:
In this work, the numerical simulations have been performed using the SCAPS-1D simulator to study the effects of Zn(O,S) buffer layer thickness and operating temperature on the performance of p-CZTS/n-Zn(S,O)/ITO based hetero-junction solar cells. To achieve the optimal cell performances, the thickness of the Zn(O,S) buffer layer varies from 0.025 to 0.3µm and the operating temperature varies from 300 to 450K. We note that the cell efficiency is maximum for a thickness of the Zn(O,S) layer which is equal to 0.05µm. Beyond this value, the efficiency is a decreasing function of the thickness; it decreases from 22.89 to 21.92%. Since the solar panels are installed outdoors, we investigated (in the second part) the effect of operating temperature on the performance of p-CZTS/n-Zn(O,S) thin films solar cells by keeping all optimized parameters constants except the working temperature was varied between 300 and 450K under fixed irradiation light of 1000W/m2. The variations of the photovoltaic performances' parameters VOC, FF, JSC and η versus operating temperature. It has been found that the efficiency of solar cells decreases significantly with increasing operating temperatures. At operating temperatures varying from 300 to 450K, the efficiency goes from 22.89 to 8.43%. The open circuit voltage VOC also decreases with the increase of the operating temperature.

Modeling of nonlocal shift induced by adsorption in adatoms-resonator biosensor subjected to magnetic field

Mohamed Mektout, Hicham Bourouina, Yahia Maiza , Soumia Khouni, Abir Lamari

Physical Sciences Department, Normal School of Bou-Saada, Bou-Saada, 28200, M'Sila, Algeria

Corresponding author: mektout.mohamed@ens-bousaada.dz

Abstact:

The present paper models and examines the nonlocal frequency shift of an adatom-nanoresonator system under a magnetic field environment owing to atoms adsorption in the presence of the surface effect, considering the small-scale effect as well as distributed adatoms, shear distortion, rotary inertia, and magnetic field effects using the Eringen's nonlocal theory. The Lenard-Jones (6-12) potential is employed to calculate the adsorption-induced energy due to the Van der Waals (vdW) mechanism interaction for both substrate-adatom and adatom-adatom. Explicit shear force and inertia moment are obtained by the nonlocal Timoshenko beam standard equations taking into account the residual stress applied as an additive axial load. The Lorentz force generated by the horizontal vector of the magnetic field is determined using Maxwell's equations. Numerical results show that the calculated resonance frequency shift depends on each of the small-scale, adsorption density, magnetic field intensity, the volume fraction of porosity, and power law index effects. The development of outcomes illustrates that the adsorption phenomena make the nanostructure softer, emphasizing the importance of considering this factor during the computations.

Keywords: Adatom-Nanoresonator System, Magnetic Field, Small-Scale Effect, Distributed Adatoms, Functionally Graded Nanobeam, vdW Interaction, Nonlocal Elasticity, Adsorption-Induced Energy.

Modeling for the resonance frequency induced by temperature loads in FGM porous nanobeam system

Abir Lamari, Hicham Bourouina, Soumia Khouni, Yahia Maiza, Mohamed Mektout

Department of Physical Sciences, Higher Normal School of Bou-saada, Bou-saada, 28200, Algeria

Corresponding author: lamari.abir@ens-bousaada.dz

Abstact:

In this paper, we investigate the impact of temperature loads on the dynamics vibration of a functionally graded material (FGM) nanobeam structure with porosity based on the Euler–Bernoulli beam model (EBM). The developed resonance frequency expressions are derived by modifying the standard equations of dynamics beam vibration. The small-scale effect is adopted via Eringen's nonlocal theory, while the coupled governing equations are obtained and solved using the Differential Quadrature method (DQM) to determine the resonance frequency of porous FGM nanobeam with simply-supported boundary conditions. Therefore, Numerical results showed that the resonance frequency depends on each of the geometrical parameters such as the porosity distributions, porosity volume fraction, and small-scale effects as well as the temperature distribution, and power-low index. Thus, numerical results are discussed in detail for a proper analysis of the dynamic vibration behavior of FGM nanobeam systems which are of interest in the development of mass-sensing integrated devices.

Keywords: FGM nanobeam, porosity, temperature loads, small-scale effect, resonance frequency, DQM.

First-principles calculations to investigate strong half-metallic ferromagnetic and thermoelectric sensibility of New Spin gapless semiconductor alloys RhCoVX (X = Al, Ga, and In) alloys

Mohamed Lamine Belkhir, Mohamed Elsaid Sarhani , Ahmed Gueddouh

University of Laghouat

Corresponding author: ma.belkheir@lagh-univ.dz

Abstact:

New Spin gapless semiconductor alloys RhCoVX (X=Al, Ga, and In) were investigated for stability and half-metallic ferromagnetic features. Three nonequivalent structural arrangements of type I, II, and III structures are considered. Type I is described as the most stable phase for all these compounds in ferromagnetic order compared to non-magnetic order. We also demonstrate the thermodynamic, dynamic, and mechanical stability of RhCoVX by computing the cohesive energies, formation energies, phonon dispersion curves, and elastic constants. Using GGA-mBJ calculations show that RhCoVX are Spin gapless semiconductor half-metallic ferromagnets, with indirect bandgap through the altered Becke-Johnson (mBJ), Furthermore, the electrons at the Fermi level (EF) were fully spin-polarized. The total magnetic moment in these three compounds was found as an integer value of 2.00µB per formula. All calculations used the DFT based on the FP-LAPW method implemented in the WIEN2K code. The effective mass of electrons/holes is (0.167/0.385) for RhCoVAl and (0.454/0.322) for RhCoVGa and (0.604/0.242) for RhCoVIn. The semi-classical Boltzmann transport theory has been used to investigate thermoelectric properties and we found that three compounds exhibit a high Seebeck coefficient and high power factor up to 1.5 mV/K for RhCoVAl and 1.25 mV/K for RhCoVGa.

Structural and electronic properties of indium phosphide : An ab initio calculations

Kenieche Daoud

Département de physique, faculté des sciences exactes et informatique, université de Jijel

Corresponding author: daoud.kenieche@univ-jijel.dz

Abstact:

In this work, the structural and electronic properties of indium phosphide (InP) were studied and interpreted using ab initio calculations. The calculations were based on the generalized-gradient approximation (GGA) level with STO-3G basis set coupled with large unit cell method (LUC). The Gaussian 03 computational packages has been employed to compute some physical properties such as equilibrium lattice parameter, energy gap, valence and conduction band width, total energy, cohesive energy and density of state (DOS). The obtained results for the band structure and the density of states show that the compounds has a direct gap at room temperature. The lattice parameter as well as energy gap have been calculated and discussed. Our calculated values have shown conformity with the experimental data. Comparing our results with the available experimental and theoretical data in the literature showed a very good agreement.

Keywords : Ab initio , Density functional theory, Indium phosphide.

Study the effect of adsorption and holes network on nanobeam vibration using non-local elasticity approach

Yahia Maiza[1], Hicham Bourouina[1], Mohamed Mektout[1], Abir Lamari[1], Soumia Khouni [1]

[1] *Physical Sciences Department of Higher Normal School of Bou-Saada, Bou-Saada, 28200, Msila, Algeria*

Corresponding author: maiza.yahia@ens-bousaada.dz

Abstact:

In order to provide an addition to the field of Nanomaterials, the frequency shift calculation was addressed to study and model the vibration of the gold nanobeam system, which is characterized by square and periodic holes along the nanobeam, in addition to the adsorption of hydrogen adatoms on its surface, using both the shear beam model (SBM), which takes into account the effect of shear deformation and Euler beam model (EBM) were developed by modifying the coupled system equations as well as taking into account small-scale behavior using Eringen's elasticity theory. The adatom-substrate energy and the adatom-adatom energy were introduced using van der Waals (vdW) interactions under the Lennard-Jones potential (6–12) to determine the overall energy shift. The frequency shift of the H/Au(100) system was calculated, which was shown to depend on the nanobeam dimensions, size and number of holes as well as the adsorption density and mode number. These results have been interpreted in detail towards the appropriate design of mass detection and Biosensor devices and their applications in Nanotechnology.

Exploring the optical bound state in the continuum in periodic 1-D dielectric grating

Djemaiai Lylia, Mezeghrane Abdelaziz, Belkhir Abderrahmane And Baida Fadi Issam

Université Mouloud Mammeri de Tizi-Ouzou

Corresponding author: lylia.djemaiai@ummto.dz

Abstact:

In the recent years, advances in Nano-fabrication technologies have led to the rapid exploitation of Bound states In the Continuum (BICs) in photonics, enabling real applications in the fields of sensors, lasers and filters. BICs can eliminate radiation losses to theoretically achieve an infinite quality factor Q. However, in practical applications, due to the finite extent of the real structures, the absorption properties of the material and other intrinsic and external perturbations, BICs turn to quasi-BICs modes. Such resonances have been used to achieve very high quality factor resonances in many photonic structures.

In this Work, based on Finite-Difference Time-Domain (FDTD) and Fourier Modal Method (FMM) simulations, we have systematically studied the existence of particular so-called symmetry protected BIC modes (SP-BIC) in a basic 1D-periodic grating. These SP-BIC can be excited as a consequence of an intrinsic (by the special discretization in the FDTD algorithm) or extrinsic breaking (by variation of the angle of incidence) of the symmetry. Our results show the excitation and propagation of two modes, classical GMR (leaky mode) and SP-BIC mode along the grating with a high Q-factor. Furthermore, the discussions are based on the characterization of these special modes in case of a grating consisting of an infinite number of periods in both normal and oblique incidence.

Keywords: SP-BIC mode; Classical GMR mode; FDTD and FMM methodes.

Ab-initio calculations of the defect effect in helical chain on the density of states for t-Se

Mekahlia Mahira

laboratoire de physique appliquée et théorique, l. P. A.t, université laarbi tebessi tébessa, algérie

Corresponding author: mekahlia.maha.2014@gmail.com

Abstact:

In this research, we study the density of states of trigonal Se (t-Se) and t-Se containing a defect (t-Se(D)) in the dihedral angle using the WIEN2k code based on the density functional theory (DFT). Based on structural properties, the t-Se(D) has the same structural parameters as the t-Se ones except a change in the dihedral angle at the position of the defect. The density of states show the semiconductor nature of the both t-Se and t-Se(D), it also turns out that the introduction of the defect decreases the gap by the creation of states in the conduction band edge. By a defect, the p states region for Se atoms change its density in such way it become more spread in energy and its upper peaks drop, this is mostly due to the change in the p-orbital. Hence, intra-chain interactions have a role in determining the gap value; this is proven by the defect in ϕ. The control of the gap by the defect opens real opportunities for applications like photovoltaic and optical storage.

Elastic and structural properties of copper carbonate CuCO3 : A nanoscale simulation study

Benazzouz Brahim Khalil

Department of Civil Engineering, LMgCE, Ecole Nationale Polytechnique (ENP), El Harrach, Algiers, Algeria

Corresponding author: brahim_khalil.benazzouz@g.enp.edu.dz

Abstact:

Carbonates minerals (with a general formula of XCO3 where X represents one or more metal ions +2) properties have been thoroughly studied and have found many applications in engineering fields. This study aime to exhibit more properties of a copper carbonate (CuCO3) from a single-crystal. The literature data, copper carbonate nanoparticles are produced through electrochemical synthesis, synthesized inorganically, biomineralization, and other process. Basic copper carbonates have been also studied for their chemical and physical properties. An atomistic simulations based on energy minimization technique were carried out using an interatomic interactions potential to describe the crystal structure of copper carbonate. The calculated structural and elastic properties including the elastic constants of copper carbonate under normal conditions are presented.

Keywords : copper carbonate, elastic constants, atomistic simulations, single-crystal.

Oxide Thickness Variations and Their Effects on VDMOS Transistor Performance

Ben Othmane Djemâa, Nozha El Ahlem Doghmane, Faiza Hadji, and Abdellaziz Doghmane

Laboratoire des Semi-conducteurs, Département de Physique, Faculté des Sciences, Université Badji-Mokhtar, Annaba, B.P 12, DZ-23000 Algeria.

Corresponding author: benothmanedjemaa96@gmail.com

Abstact:

This study explores the impact of oxide thickness variations on the performance of Vertical Double-Diffused Metal-Oxide-Semiconductor (VDMOS) transistors. The oxide layer within the VDMOS structure is a critical factor influencing device characteristics. This research investigates how changes in oxide thickness affect on the performance parameters of VDMOS transistors such as Drain current (IDS), Ion/Ioff ration, and threshold voltage (Vth). Results indicate that as the oxide thickness increases from 100 to 250 nm, the Ion/Ioff ration increases from 1x107 to 1.14x108, and there is a noticeable rise in the threshold voltage from 3.125 to 3.43 V. The findings extracted from this investigation offer crucial insights for refining both the design and fabrication processes of VDMOS transistors. By grasping the intricate implications of oxide thickness variations, engineers are empowered to customize device properties according to precise application demands. This understanding contributes significantly to enhancing the efficiency and reliability of power electronic systems reliant on VDMOS technology.

Keywords: a-ITZO TFTs, SiO2/HfO2, Al2O3/HfO2, Silvaco, Electrical parameters.

Multi-layer system and the phase diagrams of a spin-1 Blume Capel model with non-equivalent planes

Amel Benmansour, Smaine Bekhechi, Nabil Brahmi

Laboratory of Theoretical Physics, Faculty of Sciences, University of Tlemcen, BP119, Algeria.

Corresponding author: amel.benmansour93@gmail.com

Abstact:

We use the Monte Carlo simulation method for the study of the magnetic properties of a spin-1 Ising multilayer with antiferromagnetic interlayer couplings and ferromagnetic intralayer couplings. The system is composed of non-equivalent planes A and B, with B being site-diluted. The occurrence of a compensation phenomenon is observed, as well as the compensation temperature, below the critical point T_c. We discuss the effect of each of the Hamiltonian parameters on the behavior of the system; our results are presented in the form of phase diagrams where the compensation phenomenon is present or absent. Our results are comparable with those found in multilayer with spin-1/2 and dilution, as well as with trilayer without dilution. This model exhibits disordered paramagnetic phases and ordered ferromagnetic phases separated by a transition line, which changes from a discontinuous phase transition to a second-order transition at the tricritical point that depends on spin concentration P.

Excluded volume effect in 1D confined nanoparticles with permanent magnetic dipoles

Sofiane Meddour, Lila Bouzar, René Messina
Materials Physics Laboratory, University of Science and Technology Houari Boumediene (USTHB)
Corresponding author: lila.bouzar@usthb.edu.dz

Abstact:
We are interested in the behavior of supra-paramagnetic nanoparticles subjected to a magnetic field and a 1D confinement. We are interested in the case where the magnetic field is perpendicular to the confinement axis such that the dipole-dipole interaction is purely repulsive. This repulsive interaction induces an excluded volume effect, i. e., a behavior similar to that of hard spheres. By studying the pair correlation function, we establish a mapping between these dipolar particles and the behavior of hard spheres, thus allowing us to obtain a relation between the radius of the excluded volume and the intensity of the magnetic coupling. This research may be of interest for biomedical applications. Our findings may hold potential significance in biomedical contexts, where magnetic nanoparticles are used as carriers within blood vessels.

First principles study of structural, mechanical, electronic and optical properties of Hulf-Heusler LiCaN

Baizid Abdelhak, Azzeddine Mokadem, M'hamed Guezzoul, M'hammed Bouslama

Laboratory of materials (LABMAT), National Polytechnique School (ENP) of Oran, BP 1523 Oran Mnaouar, Oran, Algeria.

Corresponding author : baizid1abdelhak@gmail.com

Abstact:

In this study, we investigate the structural, mechanical, electronic and optical properties of LiCaN Hulf-Heusler semiconductor compound using the full potential linearized augmented plane wave (FP-LAPW) method implemented in Wien2k. The obtained equilibrium structural parameters are in good agreement with available results. The bulk, shear and Young modulus, Poisson's ratio, Lamé coefficients and Debye temperature have been calculated. The elastic parameters display that LiCaN is of brittle behavior and stable mechanically. The calculated band structures indicate that LiCaN is a semiconductor with indirect band gap of 3.64 eV. The optical properties based on the real and imaginary part of dielectric function (and), the refractive index , the extinction coefficient, the reflectivity, the coefficient of absorption and the electronic loss energy function are calculated and discussed in detail. These properties make LiCaN interesting and allowing to LiCaN to be appropriate to photovoltaic applications.

Numerical Modeling of the Effect of ZnGeN2 Layer in the MQW Active Region of InGaN/GaN Light-Emitting Diodes

Samira Laznek
Université Mohamed Khider Biskra
Corresponding author : samira.laznek@univ-biskra.dz

Abstact:
Many approaches have focused on reducing the indium content of LEDs by inserting other layers such as ZnGeN2. This paper discusses the effect of the ZnGeN2 layer inserted into the wells of type-I GaN/InGaN QWs LEDs on efficiency. Simulations are carried out using the Silvaco TCAD simulator at 300K. Firstly, the new structure is compared to the standard type-I LEDs based on InGaN. Then, we highlighted the impact of the number of quantum wells and the molar fraction in the wells of ZnGeN2/InxGa1-xN type-II LEDs. Changing the molar fraction in wells (0.2, 0.18, and 0.16) affect slightly the electrical and the optical characteristics with extending of wavelength. Besides, increasing the number of wells creates spontaneous green and red emissions and improves all electrical and optical characteristics of ZnGeN2/In0.16Ga0.84N type- II quantum wells LEDs.

Exploitation of the resonance shift of the GMR in the communication range

Sabrina Mesli, Mahdi Hamidi, Abderrahmane Belkhir , Omar Lamrous And Fadi Issam Baida
Université Mouloud Mammeri de Tizi-Ouzou
Corresponding author: sabrina.mesli@ummto.dz

Abstract :
Since the early theoretical work of Wang and R. Magnusson, leaky mode, or Guided Mode Resonances (GMRs), have been the subject of increasing attention, due to their interesting optical properties that make them good candidates for various applications such as bio-detection. GMR dielectric structures are characterised by their high sensitivity to variations in the refractive index of the external medium and by the fineness of their resonance peaks, which characterise low optical losses, compared with plasmon resonances (SPR), which are specific to metal-dielectric structures and are characterised by wider
resonances.
In this work, using a calculation code developed by our research team and based on the FDTD method (Finite-Difference Time-Domain) method, we will present a strategy that enables a GMR resonance peak to be moved to another detection region without unduly attenuating detection performance in terms of Sensitivity S and Figure of Merit FOM. The first characterises the shift in the spectral position of the resonance ($\Delta\lambda$) generated by a variation in the refractive index of the detection medium (Δnc). The sensitivity defined by the relationship, the greater shift in resonance for a small perturbation in the refractive index of the detection medium. The second characterises the possibility of measuring resonance wavelength shifts with greater precision. It is defined by the relationship where is the half- height width of the resonance band.

Structural, electronic and optical properties of III-nitride alloys: First principle Calculation

Ouchene Bochra[1], Meradji Hocine[2], Ghemid Sebti[2]

[1] *Laboratoire des Nanomatériaux, Corrosion et Traitements de Surfaces, Université Badji Mokhtar, Annaba, Algeria.*

[2] *Laboratoire de Physique des rayonnements, Université Badji Mokhtar, Annaba, Algeria.*

Corresponding author: bouchraphysique15@gmail.com

Abstact:

The full potential linearized augmented plane wave (FP-LAPW) method has been used to investigate the structural and electronic, optical properties of III-nitride alloys. The calculations are conducted using density functional theory (DFT). Our selections were the standard generalized gradient approximation (GGA) and the (mBJ) approximation. The Wien2k code was used to perform the calculations. We concurred that the results were reasonable when compared to experimental and theoretical data.

The III-nitride alloys such as InN and AlN are becoming increasingly popular due to their potential use in optoelectronic and high power/temperature electronic devices, like light-emitting diodes and laser diodes. Photodetectors that detect solar blindness and heterostructure field effect transistors.

Key words: : optical properties , FP-LAPW, DFT, InN , AlN.

Preparation and study of The electronic structure of LaMnO3 nano-crystalline LMO magnetic perovskite

Djellali Brahim Said, Boussendel Abdelmadjid
Higher Normal School of Bou-Saada Msila , Algeria
Corresponding author: djellali.brahimsaid@ens-bousaada.dz

Abstact:
The nano-crystalline LaMnO3 magnetic perovskite powders were synthesized by the sol- gel method from minerals nitrate, obtained powders calcined at 700 to 1100 °C by a step of 100°C. In order to investigate the effect of sintering temperature on the crystalline structure, X-ray diffraction is then used with the Rietveld refinement to obtain the lattice parameters, space group, and the average crystallite size obtained by the FullProf Package equation. We show that samples sintered at 700 to 800 are essentially orthorhombic structures (Pnma 62). while those sintered at 900 to 1100 °C are rhombohedral structures (R-3C 167). Full-potential linearized augmented plane wave (FP-LAPW), implementation of the density functional theory calculations (DFT), show that while an orthorhombic structure is the ground state structure, a rhombohedral structure is also a stable structure with a barrier energy (67 meV)
equivalent to 850 °C. A scheme for a possible structural transition from different crystalline phases is suggested. The optimum structure for each phase is calculated by optimizing the energy versus the volume of that phase and Calculation of DOS and Band Structures for a Compound Using the VASP Code

Exploitation of metal nano structures for the study of surface plasmons in periodic lattice

L. Dehbi, A. Belkhir , A. Mezeghrane
Laboratoire de Physique et Chimie Quantique, Faculté des Sciences, Université Mouloud MAMMERI, BP 17 RP, 15000 Tizi-Ouzou, Algeria
Corresponding author: dehbi.lynda@yahoo.fr

Abstract:
We have studied the occurrence of collective resonances due to lattice effects, commonly referred to as lattice plasmon resonance. The structure studied consists of metal nanoparticles arranged in a square lattice. The lattice pitch is chosen so that lattice effects are observable. Maxwell's equations are solved using the finite-difference time-domain (FDTD) method, taking into account the dispersion of the metals studied in the optical range. The results show that the resonance attributed to individual nanoparticles is red-shifted as the grating pitch becomes larger. Resonances attributed to the grating effect appear at shorter wavelengths and exhibit a narrower profile than those of individual nanoparticles.
This study focuses on the generation of higher orders of diffraction in a plasmonic structure. When metal nanoparticles are arranged in a periodic grating with a period of the order of the nanoparticle resonance wavelength, an additional resonance to the plasmon resonances of the individual particles is generated.

Study of a silver cone-shaped biosensor for protein detection

Bensaid Cylia, Djouder Madjid, Lamrous Omar
Mouloud MAMMERI University
Corresponding author: cylia.bensaid@fs.ummto.dz

Abstact:
Traditionally, markers are used to study protein behavior. This has a major drawback, as markers influence the interaction of a protein with its environment. To avoid measurement interfering with protein behavior, current research is focusing on auto-fluorescence. This involves exciting the protein's fluorescence with UV laser radiation. The difficulty lies in the very low intensity of the fluorescence when the protein concentration is lowDans l'article [1], les auteurs présentent un capteur en forme d'un cône munis d'un orifice sur son sommet. Il est fait d'une couche d'aluminium de 100nm sur un substrat en verre. Dans notre travail, on étudie numériquement avec COMSOL Multiphysics l'effet d'une couche en argent et l'effet des paramètres géométriques sur le facteur de Purcell et sur la puissance de sortie du rayonnement. In article, the authors present a cone-shaped sensor with a hole at the top. It is made of a 100nm aluminum layer on a glass substrate. In our work, we use COMSOL Multiphysics to study numerically the effect of a silver layer and the effect of geometrical parameters on the Purcell factor and radiation output power.
Initial results are encouraging, with Purcell factors ten times greater than with the aluminum layer. We have also noted the possibility of selecting the detection range in wavelength, which was not possible with the aluminum layer.

Key words: Cone-shaped biosensor, Purcell factor, Emitted power, Comsol Multiphysics.

BaTiO3@Au nanoparticle-mediated photothermal therapy for subcutaneous tumors: A numerical analysis

Daoudi Chouaib, Brioua Fathi, Belmerabet Roqiya
University of August 20, 1955 Skikda
Corresponding author: ch.daoudi@univ-skikda.dz

Abstact:
Gold nanoparticles (AuNPs) are recognized as promising cancer therapy agents because of their distinctive physicochemical and optical properties. This paper introduces a computational model that elucidates the mechanisms of damage induced by BaTiO3@Au nanoparticles on subcutaneous tumors. We employ a finite element method, built explicitly in COMSOL Multiphysics, to investigate the interactions between BaTiO3@Au nanoparticles and tumor microenvironments. We assess the spatial distribution of temperature increase within the tumor tissue and predict the extent of cellular damage by considering the impact of irradiation type, volume fraction of nanoparticles, laser intensity, and irradiation time. The insights derived from our computational model provide valuable guidance for designing and optimizing anticancer treatments utilizing metal nanoparticles. The findings of our study add to the progress of nanoparticle-based cancer therapy and provide novel opportunities for targeted treatment of tumors.

Excitation of hybrid plasmonic modes in arrays of metallic nanostructures

M. Braik, A. Belkhir, N. Felidj
Université Mouloud Mammeri de Tizi Ouzou
Corresponding author: Macilia.braik@ummto.dz

Abstact:
Metallic nanostructures (NSs) support plasmonic surface lattice (SL) resonances resulting from long-range interactions when assembled in periodic arrays. Compared to localized surface plasmon (LSP) resonance, SL resonance from nanoparticle (NP) arrays has much narrower optical spectrum features. In the present work, we demonstrate the possibility to generate a hybridization of surface lattice (SL) resonances by exciting grazing order diffrac- tion within the metasurface similar to the hybridization of LSP resonances observed in short- range interactions. This hybridization leads to the emergence of bonding and anti-bonding modes. The anti bounding mode results in a dipole moment which is almost zero due to out-of phase dipoles oscillations between the NPs leading to a much narrower spectral linewidth. The designed plasmonic platforms are made of binary arrays with unit cells consisting of two gold discs of different diameters. We demonstrate the possibility to maximise or cancel the in- teraction between the hybridized SL resonances by simply controlling the distance between the particles. Our experimental results are supported by FDTD calculations. The hybridization of SL modes results in much richer hybridization scenarios in terms of wavelength and quality factor control compared to the hybridization of LSP in a short range configuration. It offers possibilities to design innovative optical devices with highly flexible tenability.

Theoretical investigation on orange-emitting cyclometalated platinum (II) complexes containing organosilyl/ organocarbon-substituted 2-(2-thienyl)pyridine ligands

Hadj Mezouar

Laboratory of Chemistry: Synthesis, properties and applications (LCSPA), Faculty of Sciences, University of Saida - Algeria

Corresponding author: hadjmezouar29@gmail.com

Abstract:

In this work; we studied the structural and optical properties and spectroscopic features of the two complexes Pt1 and Pt2 using DFT and TD-DFT methods level with the hybrid functional (B3pw91) and we have used the base set LANL2DZ . The optical properties results UV/VIS (absorption and emission) depict a good agreement with the experimental data. The electronic and geometrical structures of the ground state (S0) and the first triplet excited state (T1) have been analyzed and compared .To explicate the electronic behavior of molecule, complete bond analysis was executed using natural bond orbital (NBO) and Frontier molecular orbitals (FMOs). LLCT character dominates the low-lying singlet excited states. Phosphorescence wavelengths of the studied complexes were calculated vertically and adiabatically. The adiabatic methods are more accurate Phosphorescence spectra were simulated taking into account the vibronic coupling using FC/AH and FC/AS approaches. The normal modes involved in phosphorescence maxima were identified; analyzed and assigned to the observed emission maxima.

Keywords: TD-DFT, Schiff base, phosphorescence

Analysis of the Impact of Core-Shell Nanofluid Hybrids on Natural Convection

Farida Iachachene, Hanane Cheradi ,Louiza Achab and Malika kabache

UMBB

Corresponding author: f.iachachene@univ-boumerdes.dz

Abstract:

This study investigates natural convection in a square cavity containing a hybrid nanofluid. The aim is to analyze the impact of core-shell nanoparticle hybrids on heat transfer. Through numerical simulations, we will examine the influence of the shell's nature on that of the core, as well as their impact on heat transfer. The results aim to provide essential information to enhance heat transfer applications using these specific nanofluids.

DFT and comparison study of pure and M-doped SnO2 Structure

Imene Saoula, OuahabAbdelouhab, Chahinez Siad
department de physique , Faculty of sciences
Corresponding author: imene.saoula@univ-biskra.dz

Abstract:
This study investigates the doping of the rutile structure of SnO2 with alkaline earth elements denoted as 'M' (potentially Ca, Sr, or Ba) at both low (4.16 at %) and high (8.33 at %) atomic ratios. In the former, 'M' atoms substitute 'Sn' atoms located at the (0; 0; 0) position within a (2x2x1) supercell, while in the latter, the substitution occurs within a (1x1x2) supercell. The computational framework employed herein relies on the CASTEP code, utilizing density functional theory (DFT). Initially, geometry optimization for a 1x1x1 cell is conducted, involving cut-off energy optimization (800 eV) and K-point optimization (kx=8; ky=8; kz=10). Subsequently, structural optimization for 2x2x1 and 1x1x2 supercells is carried out, revealing a consistent increase in lattice parameters and cell volume with rising atomic ratio. Analysis of the band structure confirms that both pure and M-doped SnO2 exhibit a direct band gap, which narrows as the atomic radius increases, irrespective of the doping ratio. Finally, optical properties are explored, revealing an enhanced absorption coefficient (α) in M-doped SnO2 compared to pristine SnO2. The observed variation in absorption edge aligns with changes in the band gap, demonstrating a systematic relationship between absorption edge and band gap**.**

Investigation of the stability of 1, 2, 4-triazole by Rhenium complexes using the DFT method

Boukertouta Ghadir, Seridi Achour
Laboratory of physical chemistry, University 8 May Guelma, Algeria.
Corresponding author:boukertouta.ghadir@univ-guelma.dz

Abstract:
1,2,4-triazoles are interesting compounds due to their diverse application; they are attracting considerable interest as targets for medical and pharmaceutical applications. Rhenium complexes exhibit considerable cytotoxicity towards cancer cells, and these complexes are being used in explored anti-cancer therapy candidates. Rhenium complexes have several advantages over conventional organic drugs currently used to treat cancer. In this study, stable complex between a 1,2,4triazole derivative and tricarbonyl rhenium is studied theoretically, using Gaussian 09 and the DFT method. The free ligand is optimized with the hybrid function B3LYP and 6-31G(d) basis set and the complex with the mix bases set of B3LYP-LanL2DZ/6-31G(d). Different parameters were calculated including frontier molecular orbitals energies, reactivity indexes and molecular electrostatic potential allowed us to locate the sites of nucleophilic and electrophilic attack. Further data such as vibrational frequencies and UV-VIS spectra of the free ligand and the complex.

NiO's Physical Properties: A Study Based on First Principal Calculations for Solar Cell Application

Fairouz Chouit, Hayet Benzerouk, Asma Boussaha, Abdelaziz Drici
Faculty of Technology , Skikda University
Corresponding author: f.chouit@univ-skikda.dz

Abstract:
Transparent conducting oxides (TCO) are of special importance to solar cells; letting light into the solar cell to convert light into energy while acting as collectors for converted energy. A good TCO is one that possesses high electrical conductivity combined with a low absorption rate in the visible and high reflection in the infrared. Nickel oxide is an attractive material due to its chemical stability. This compound has a set of physical properties (optical, magnetic properties, etc.) likely to use it in numerous applications in the field of electronics and optoelectronics. In this work, we have studied the structural properties, elastic constants, and mechanical properties, using the first principals' calculations based on FP-LAPW method (Full Potential Linear Augmented Plane Wave) within DFT (Density Functional Theory). The obtained values of elastic constants proved that the studied material is mechanically stable; it is shown that the NiO compound have ionic bonding dominantly. The value of anisotropy coefficient A obtained at 0 GPa for our material is different to 1, thus indicating that it is elastically anisotropic. The value of the B/G ratio is 3.99; the material studied presents ductile behaviour which makes it a good candidate for optoelectronic devices.

Molecular docking and ADMET study of a phenolic Schiff base

Manal Chettibi, Saida Seridia, Marwa Benmabrouka.
Laboratory of physical chemistry, University 08 May 1945, BP401, Guelma 24000, Algeria.
Corresponding author: chettibi.manal@univ-guelma.dz

Abstract:
In this study a Schiff base ligand, namely 4-{(E)-[(4-hydroxyphenyl)imino]methyl}-2-methoxyphenol, was synthesized and characterized. The ligand was then docked with two different lung cancer receptors, identified by their Protein Data Bank (PDB) codes: 1x2j and 5xnv. Molecular docking studies were conducted to investigate the potential anticancer properties of the ligand using AutoDockVina. The results obtained from these studies can provide valuable insights for the development of novel cancer therapies. The drug candidate's potential efficacy, safety, and pharmacokinetic profile were assessed using ADME-Tox properties. Additionally, the likelihood of the molecule becoming a drug was evaluated using the Lipinski's rule.

Keywords: Schiff base, Lung cancer, Molecular docking, ADME-Tox and Lipinski's rule.

First-principles study of structural, electronic and magnetic properties of Ti doped calcium selenide (CaSe)

Amina Aiche, Hadjmoulay Ahmed Mazouz
University MouloudMammeri of TiziOuzou, Physics department, Faculty of sciences
Corresponding author: amina.aiche@ummto.dz

Abstract:
We have performed a first-principles study to investigate the electronic structure and the magnetic properties of calcium selenideCaSe semiconductor doped with transition metal impurity Ti using the full-potential linearized augmented plane wave (FP-LAPW) approach to the density functional theory (DFT). Total energy calculation allowed us to determine the ground-state parameters, namely the lattice constant, the bulk modulus ant its first pressure derivative. The electronic properties are calculated using both the generalized gradient approximation proposed by Wu and Cohen (GGA+WC) and the Tran Blaha modified Becke-Jonhnson (GGA-TBmBJ) for the exchange and correlation potential. The studied compound is found to be half-metallic ferromagnets with a total magnetic moment of 2 Bohr magneton. Also, we reported the calculated exchange constants and the band edge spin splitting of the valence and conduction bands. The objective is to seek new half metallic ferromagnetic material for an application in the new emerging field of spintronics and the studied compound is suitable candidate for such application.

Exploring Gas Influence on X-Ray Profiles and Optimizing Characterization Conditions at the Al/Ag Interface in ESEM

Lateb Nouria, Mansour Omar , Kadoun Abd-Ed-Daim,
Laboratoire de Microscopie, Microanalyse, et Sciences des Matériaux (L2MSM), Faculté des Sciences Exactes, Université Djilali Liabès, 22000 Sidi Bel-Abbès, Algeria.
Corresponding author: nouria_lateb@univ-boumerdes.dz

Abstract:
This study delves into the intricate interplay between electrons and materials within the context of the environmental scanning electron microscope (ESEM), particularly examining its impact on X-ray profiles at the Al/Ag interface. Through Monte Carlo Simulation, we explore the correlation between skirt radius and gases (specifically, H2O and N2), shedding light on how different gases influence this relationship. Moreover, we dissect the influence of gas properties, accelerating voltage, and pressure on the secondary X-ray fluorescence phenomenon, aiming to pinpoint the optimal imaging pressure for observing the Al/Ag interface. Our experimental findings highlight the potential enhancement of X-ray resolution through pressure reduction or the use of gases with lower atomic numbers. Our analyses underscore water vapor as the most conducive environmental imaging gas, effectively bridging the gap between microanalysis profile resolution and the X-ray fluorescence and absorption effects at the Al/Ag interface.

Keywords: ESEM, Monte Carlo Simulation, X-ray resolution, EDS profile, skirt radius, Interface.

Exploring the Influence of Electron Irradiation (A Comprehensive Investigation with Optical Microscopy and MonteCarlo Simulation)

Lakhdari Amani Sabrine[1], Benarroudj Abdelkrim [1]and Zoukel Abdelhalim[2]

[1]*Materials Laboratory for the Application and Valorization of Renewable Energies (LMVER), Laghouat, Algeria*

[2]*Physico-chemical analysis technical platforms. CRAPC, Laghouat, Algeria*

Corresponding author: as.lakhdari@lagh-univ.dz

Abstract:

In our study, we delved into examining the impact of electron irradiation on polymers through a combination of simulation and experimental investigation. To begin with, we aimed tounderstandthescaleanddepthoftheinteractionusingtheMonteCarlosimulationprogram "Casino." The simulation involved the use of 100,000 electrons with electron energies of 5 kilovolts and 25 kilovolts. Subsequently, we transitioned directly to the experimental phase. Here, we irradiated the sample using a scanning electron microscope, followed by utilizing an optical microscope as a tool to observe surface topography. This allowed us to visually identify any changes that occurred, ensuring accurate translation of our findings without errors.

Keywords: Spintronics ,PMMA ,polymers ,MO, SEM, CASINO.

Spin dynamics and surface magnons in antiferromagnetic monoxide

M. Boucherrab [1], B. Bourahla [1]

[1] *Laboratoire de Physique et Chimie Quantique, Université Mouloud Mammeri, 15000, Tizi-Ouzou, Algérie.*

Corresponding author: mali_bou@yahoo.fr

Abstract

A theoretical model to study the spin excitations in the transition metal monoxides of the first series which adopt a structure of the NaCl type. The model is mainly used to analyze the antiferromagnetic monoxide network of spins, using the matching method theory. The magnon spectrum is determined by numerical calculations based on the Landauer-Buttiker formalism of the scattering matrix.

Our simulation results show the interference effects ¨ between magnon states of the monoxide continuum and the localized magnon modes created by the surface region with Fano resonance characteristics. Additionally, The magnetic spectra are determined and discussed according to the different parameters characterizing the structures under study.

Keywords: Antiferromagnetic monoxides, Spin waves; Matching method, localized spin states.

Phonon transmission via an atomic interface

M. Boucherrab [1], B. Bourahla [1], R. Tigrine [2]
[1]*Laboratory of Physics and Quantum Chemistry, Faculty of Sciences; M. Mammeri University, B.P.N°17 RP, Tizi-Ouzou, Algeria.*
[2] *Univesity Ahmed Draya, Adrar Algeria.*
Corresponding author: mali_bou@yahoo.fr

Abstract :
In this work, we study the vibrational properties of the atomique interfaces. The main interest is to understand the mechanisms for the scattering and propagation of elastic waves through the atomic nanostructures inserted into hexagonal structures. Our study is based on the application of the theoretical matching method and Green's theory functions in the frame of harmonical approximation, in order to describe, in details, the localized vibrational properties in behavior of the perturbed domain. The transmission and reflection coefficients, the total conductance, and the state densities in presence of different homogeneities were determined as function of physical quantities characterizing the system model. Our results show that the transmission and the reflection coefficients depend on the interferences between the diffused elastic waves by the defect. In addition, the interaction between the states of the scattering and the localized vibration states at the defect give raise the Fano resonances and Fabry-Perot oscillations on the different properties like the conductance and state densities.

Keyword: Interface dynamic, Nanostructures, Elastic waves diffusion, Densities of state.

The production of solar energy: a study by DFT and TD-DFT

Mohammed El Amine Zair[1], Hafida Chamouri[1,2]

[1]*Laboratoire de Thermodynamique Appliquée et de Modélisation Moléculaire (LATA2M) N°53, Département de Chimie, Faculté des Sciences, Université A. BelkaïdUniversity, B. P. 119, Tlemcen, 13000, Algeria*

[2]*Ecole Supérieure des Sciences Appliquées, ESSA-Tlemcen, 13000, Tlemcen, Algeria*

Corresponding author: mohammedelaminezair@gmail.com

Abstract:

The use of fullerene-based carbon materials in perovskite solar cells offers advantages such as highere fficiency and improved stability. DFT and TDDFT modeling will be used and the geometries of the structures will be optimised by Gaussian 09. However, questions remain about fullerene doping and it seffect on solar cell efficiency. This perspective examines the progress made in understanding the behaviour of fullerenes in perovskite solar cells, looking in particular at how full erenescanim provehybrid photovoltaic cells and whether doping fullerenes with perovskite improves cell efficiency. It also examines why perovskite and fullerene solar cells are more efficient than simple organic photovoltaic cells.

Keywords : DFT, TD-DFT, PCBM, pérovskite.

Review on Nanomagnetic Materials: Properties, Methods, and Applications

Salah Blizak
Department of physics, Faculty of sciences, University Mohamed Boudiaf of M'Sila, Algeria
Salah.blizak@univ-msila.dz

Abstract:
Nanomagnetic materials have emerged as a focal point of interdisciplinary research due to their unique magnetic properties and diverse applications across various fields. This review provides a comprehensive overview of nanomagnetic materials, encompassing their fundamental properties, synthesis methods, and practical applications. The intrinsic characteristics of these materials, such as high surface-to-volume ratios, superparamagnetism, and size-dependent magnetic behavior, are discussed in detail. Various synthesis techniques, including chemical vapor deposition, sol-gel processes, electrodeposition, and ball milling, are critically analyzed with respect to their advantages, limitations, and scalability. Furthermore, the review highlights the wide-ranging applications of nanomagnetic materials in data storage, biomedicine (e.g., drug delivery, hyperthermia, and imaging), catalysis, environmental remediation, and energy conversion/storage systems. Challenges associated with the stability, toxicity, and large-scale production of these materials are also addressed, along with potential strategies to overcome them. Finally, this review concludes by outlining future research directions aimed at advancing the design, fabrication, and utilization of nanomagnetic materials for emerging technologies.
Keywords : Nanomagnetic materials, magnetic properties, superparamagnetism, Nanomagnetic applications

First-Principles Calculations on Structural and Electronic Properties of SrTe compound with LDA approximation at different pressure

Daho Salah Eddine and Mehtougui Nabila
Affiliation of the participant: Hassiba Benbouali University, Chlef, Algeria
Corresponding author: dahouhbc@gmail.com

Abstract :
Our calculations are investigated the structural and electronic properties of SrTe compound, the density-functional theory within the (LDA) approximation is employed using The full-potential muffin-tin orbitals (FP-LMTO) method. The equilibrium lattice parameters, bulk modulus and its pressure derivative were investigated. Band structures character of SrTe compound is determinates.

TABLE OF CONTENT