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FACULTY OF EXACT SCIENCES

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1ST-ICRAMPCS 2024



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PREAMBLE

The First International Congress on Recent Advances in Mathematical, Physical, and Chemical Sciences is a prestigious global gathering that brings together researchers, scientists, academicians, and industry professionals. The Congress serves as a platform to showcase and discuss the latest advancements, discoveries, and innovations in mathematical, physical, and chemical sciences. Participants exchange knowledge, ideas, and insights, while eminent scientists deliver plenary talks and keynote lectures. These sessions inspire new research directions and offer valuable perspectives. Overall, the Congress fosters scientific collaboration, knowledge dissemination, and contributes to societal progress through advancements in these fields.

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Conferences

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Spectral Theory of Multivalued Linear Operators



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The subject of this exposed is the study of linear relations over real or complex Banach spaces. The main purposes are the definitions and characterization of different kinds of spectra and extending
the notions of spectra that are considered for the usual one single-valued operator bounded or not bounded.

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Liaisons chimiques et interactions inter atomiques observées par les cristallographes



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La chimie, la physique, la biologie et tout ce qui nous entoure, ce que nous sommes, ce qu'on était et ce nous serions, la matière et ses états complexes, qu'elle soit vivante, morte inerte ou active…..sont régis par des arrangements électroniques appelés communément *liaisons chimiques et interactions interatomiques*.

On essaiera de regarder ces interactions à travers une fenêtre cristallographique, sachant que cette science qu'est la radiocristallographie est la première à accéder à l'infiniment petit et a permis aux scientifiques de '*voir'* les atomes et d'étudier leurs environnements électroniques formés de liaisons et d'interactions expliquant ainsi, prévoyant et déterminant aussi des propriétés physico-chimiques ou biologiques des substances.

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The contribution of Fourier analysis in developing functional materials and nanomaterials



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The development of various scientific fields is mainly centred on innovative concepts that are often based on simple ideas, but which are the result of profound reflection. The emergence of '*modern*' physical and chemical approaches and theories such as Relativity, Quantum Mechanics, Radioactivity, Plasma, Chemical Kinetics, Phase Transitions, the design of Molecular Machines, the elaboration of Quantum Dots, etc, would have been impossible without recourse to highly advanced and powerful mathematical concepts and tools. This need had already become apparent over time. For example, in the XIXth century for Electromagnetism and the contribution of partial differential equations; Statistical mechanics, whose founding father can be considered Boltzmann; or in the XXth century with the advent of Quantum Optics and the notion of wave-corpuscle duality to answer the conceptual problem of the nature of light, which has long been a source of debate and divergence within the scientific community.

Despite the fact that the approaches pursued by chemists, physicists and mathematicians are very different in nature, simply as a result of the objectives targeted by each of them, it is nonetheless certain that chemistry, physics and mathematics are intellectual disciplines that are very close, as can be evidenced not only from their history but also from their fruitful exchanges and the enrichment they have brought to one another. In this context, Fourier's analysis and series [1] and their use are the perfect illustration. Indeed, Fourier's contribution has not only revolutionised all areas of scientific research, but it has also undoubtedly had a significant impact on our daily lives (communication and signal processing, analysis techniques, medical imaging, etc.). In this contribution, I will present a few examples and applications [2-3] of the contribution of Fourier series to the development of physicochemical characterisation approaches for functional materials and nanomaterials in the fields of energy transition and renewable energies, digital transition and medicine and pharmacology.

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Hasard, déterminisme, chaos, physique quantique...le fabuleux pouvoir des Mathématiques



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Les mathématiques, avec leur langage universel et rigoureux, transcendent les frontières entre disciplines, révélant l'ordre caché du chaos, démystifiant les lois du hasard et explorant les mystères de la physique quantique. Elles sont le fil d'Ariane qui nous guide à travers le labyrinthe complexe de notre Univers.

Cet exposé consiste à apporter un éclairage, une perspective enrichissante sur le rôle central que jouent les mathématiques aussi bien dans l'expression de concepts fondamentaux à la charnière de l'épistémologie et de la métaphysique, que dans le développement des théories les plus révolutionnaires de la physique.

Le **déterminisme** et le **hasard** sont anthropocentriques, inscrits dans l'horizon des préoccupations humaines et de fait intrinsèquement liés tant à l'évolution des idéaux de la connaissance qu'au cheminement de la métaphysique.
Si le déterminisme se profile derrière les lois de Newton, le hasard n'est pas en reste. Sa rationalisation, sa formalisation a donné lieu à l'émergence de la théorie des Probabilités.

La première faille ou révolution dans la signification et la portée du déterminisme est apparue avec les **systèmes dynamiques déterministes non linéaires** dont le comportement est imprédictible, imprévisible à terme et ce en raison d'une forte sensibilité aux conditions initiales.
Ce phénomène, mis en évidence pour la première fois par Poincaré, ne signifie pas que le hasard fasse

loi, ces systèmes étant décrits par des modèles déterministes et non aléatoires même si leur état est illisible à long terme et d'apparence chaotique. Ce fait justifie le paradoxe de la formule **« chaos déterministe »** qualifiant ce type de comportement.

La seconde faille du déterminisme, et non des moindres, a été provoquée par Einstein et les fondateurs de la **mécanique quantique** en imposant un ordre nouveau s'étendant bien au-delà de la réalité observable, celui de la relativité et du quantique.
Einstein, dans son essai « Première Théorie des Quanta » constate la permanence du caractère probabiliste des prédictions de sa théorie. La formulation probabiliste devient irréductible dans la description de la réalité physique en Mécanique Quantique. La Physique Quantique est qualifiée d'**Indéterministe**. On parle alors de crise de la causalité et du principe de déterminisme mais ce dernier n'est pas mort, et pour preuve il est au cœur des fonctions d'ondes en Mécanique Quantique. Par ailleurs la théorie des **systèmes dynamiques chaotiques** conjuguée au **principe d'incertitude d'Heisenberg** fait voler en éclats tout espoir d'une possible prédictibilité ou prévisibilité.

Ainsi se posent le problème de l'écart entre le possible et le réel, et la question du rapport des mathématiques au réel.

L'univers des Mathématiques est composé de concepts et d'objets abstraits fascinants ayant une existence propre : le point, les espaces à n dimensions, l'infini, les nombres, les matrices, les champs vectoriels, les équations différentielles, les fonctions, les intégrales, la géométrie fractale, les invariant topologiques, les tresses, les nœuds, les opérateurs, la dynamique symbolique, les variétés, les attracteurs étranges...

Les mathématiciens continuent d'explorer, de développer et d'élaborer des théories toujours plus étonnantes et plus efficaces à partir de cette « matière abstraite » et ce afin que des physiciens, des chimistes, des astronomes, des épidémiologistes, des financiers, des informaticiens, des météorologues, des artistes..... s'en servent pour découvrir, décrire, comprendre et prévoir une infinie variété de phénomènes de l'Univers allant de l'infiniment petit à l'infiniment grand.

Cet exposé est une mise en lumière de la fabuleuse efficacité de la symphonie mathématique qui se trouve derrière chaque phénomène, prête à être découverte, décodée et appliquée pour le progrès de la science et de l'humanité.

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Le développement durable
‘‘La clé de l’avenir’’



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Les développements, industriel et agricole, associés à l’explosion exponentielle de la population mondiale et à l’aspiration à une vie de plus en confortable, ont conduit à l’exploitation massive, voire abusive, des énergies d’origine fossile. Une étude prévisionnelle des consommations et sources d’énergie conventionnelles, afin de mettre en œuvre une politique énergétique pour les prochaines décennies, montre sans ambiguïté que non seulement ces ressources ne sont pas inépuisables mais que par ailleurs, les diverses contraintes techniques, écologiques, sociales et politiques, viennent limiter les possibilités de couvrir l’approvisionnement énergétique mondial si la croissance des besoins reste soutenue, ce qui sera certainement le cas. De plus l’impact néfaste de ces énergies sur l’environnement (émission de GES, réchauffement climatique, et autre..) est incontestable. En effet, d’après le rapport annuel du Haut Conseil pour le Climat, l'année 2022 a été marquée par une intensification significative des conséquences du changement climatique. La température moyenne de la Terre a enregistré une augmentation de 2,9°C au cours de ces dernières décennies, et les précipitations ont quant’à elles diminué de 25% pendant la période de 1991 à 2020. Aussi, agir rapidement et efficacement pour trouver des solutions réfléchies à ces défis énergétiques et environnementaux actuels et qui pourraient impacter fortement, non seulement notre quotidien mais également le devenir des générations futures, voire celui de l’humanité, devient une nécessité absolue. Beaucoup d’entre nous sont convaincus que le développement durable est la clé de l’avenir ! Ils s’accordent à voir celui-ci comme une révolution de la pensée, du progrès et de la croissance, pour vivre mieux et dans le respect de la nature. De ce fait, appliquer des changements radicaux dans le mode de développement de nos sociétés (une gestion responsable et efficace des ressources naturelles, un mix énergétique plus diversifié, l’adoption de pratiques respectueuses de l’environnement), reste la seule issue à notre sécurité énergétique, à celle des générations futures et à la préservation de notre planète.

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Applications and future perspectives of innovative green technology: Supercritical fluid extraction



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Introduction and Purpose: Green extraction of bioactive phytochemicals from natural plants usually involves several separate steps and requires large volumes of organic solvents. A comprehensive subcritical and supercritical fluid extraction method using carbon dioxide and co-solvents will be presented. This new approach allows the extraction of non-polar and polar phytochemicals in many consecutive steps. In the first step after cold pressing for oilseeds, a low amount of co-solvent and a high amount of CO_2 are used to selectively extract non-polar volatile phytochemicals in a short time. Increasing the co-solvent volume in the extraction solvent up to 20% (v/v) allows the extraction of more polar compounds, including flavonoids and phenolic acids, in less then two hours. Changing the supercritical CO_2 extraction conditions does not require any manual intervention in our newly developed fully automatic device, but results in two separate fractions containing target compounds with different physicochemical properties. In this study, the developed device was investigated in terms of repeatability, accuracy, precision and greenness.

Materials and Methods: Supercritical CO_2 extraction was applied to many plant species for volatile phytochemicals and phenolic profiles. The results proved that this concept is suitable for the analysis of complex plant samples. It also reduces the consumption of toxic solvents, extraction time and manual intervention required for traditional extraction approaches while isolating different metabolite groups. Supercritical CO_2 extraction method is important due to the use of environmentally friendly, non-toxic solvents, ability to operate at lower temperatures that do not cause degradation of bioactive compounds and rapid extraction capacity. The extracts obtained showed superior properties due to their activities. In order to obtain extracts as a bioactive agent, 40 kg of the dried part was weighed and this pure and organic plant placed in tubes and extracted with supercritical carbon dioxide. Volatile components of plant extracts obtained from plant were determined with LC-MS/MS, GC-MS/MS and NMR techniques.

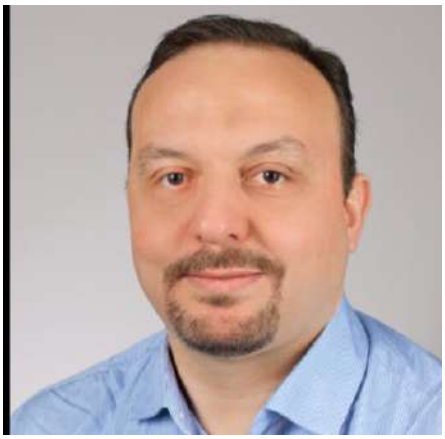
Results: According to the analysis results, many compounds were identified; terpenoids, fatty acids, flavonoids and other phytochemicals.

Discussion and Conclusion: The aim of this presentation is to provide an in-depth understanding of supercritical CO_2 extraction method and to discuss its advantages and disadvantages. The study includes specific data on various plant materials and includes details such as plant name and region, bioactive compounds or compound classes, extraction temperature, pressure, time, co-solvent used and flow rate. This study covers the investigations on the isolation of bioactive compounds and the activities of the obtained extracts.

Key Words: Plants; supercritical CO_2; LC-MS/MS; GC-MS/MS; NMR; Phytochemicals

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Stability Analysis of Boiling Water Reactors: Understanding the Dynamics of Neutrons' "Dance"



Dr. ABDELHAMID DOKHANE

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Nuclear energy remains a crucial component of global electricity generation, contributing approximately 10% of the world's total electricity and serving as the second-largest source of low-carbon energy after hydropower. Among the nuclear reactors in operation, light water reactors (LWRs) dominate, representing approximately 90% of the world's operational nuclear capacity. Boiling water reactors (BWRs), a key subset of LWRs, offer unique operational benefits by generating steam directly within the reactor core. However, their dynamic behavior under certain conditions presents challenges, particularly in the form of complex instabilities.

BWRs, though stable under normal operating conditions, can exhibit nonlinear behaviors leading to power (neutron flux) oscillations. These oscillations, categorized as global (in-phase) or regional (out-of-phase), stem from strong couplings between neutronic and thermal-hydraulic processes. Understanding and addressing these phenomena is critical for maintaining reactor safety and performance.

This presentation highlights the pivotal role of stability analysis in understanding BWR instabilities. Two complementary approaches are discussed: large system codes, which provide detailed simulations of coupled thermal-hydraulic and three-dimensional neutron kinetics behavior; and reduced-order models, which simplify system representation to focus on core physical phenomena. While system codes deliver high-fidelity quantitative analyses to identify operational exclusion zones and accurately predict system behavior, reduced-order models enable sensitivity analyses and bifurcation studies, providing deeper insights into the mechanisms driving instabilities.

Through advanced methodologies, validated models, and the integration of nonlinear dynamics and bifurcation theory, this presentation demonstrates how even the most complex instability patterns, such as out-of-phase power oscillations, can be effectively captured, analyzed, and explained.

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A generalized type of weighted proportional fractional derivatives



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There has been a growing interest in fractional calculus over the past few decades. This branch of calculus focuses on the integration and differentiation of any order, thus extending the concepts of classical calculus. One of the most notable features of fractional calculus is the existence of various types of integrals and derivatives. As a result, researchers can select the fractional derivative or integral that they believe is best suited for accurately modelling real-world problems. This work introduces an innovative type of fractional operator and explores several of its key properties. By expanding on these characteristics, we aim to enhance understanding and application in the field.

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Bioactive secondary metabolites of Algerian Asteraceae and Linaceae



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Bioactive secondary metabolites (triterpenoid saponins, triterpenes, sesquiterpene lactones polyphenols…) are found in Algerian medicinal plants belonging to Asteraceae and Linaceae. The antioxidant, antimicrobial, anti-Alzheimer, anti-diabetic, anti-inflammatory, analgesic and anticancer activities of several compounds, isolated from the studied plants, have been evaluated. A chemotaxonomic significance is also investigated.

Keywords: Antioxidant, antimicrobial, anti-Alzheimer, anti-diabetic, anti-inflammatory, analgesic, anticancer

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Numerical methods for nonlinear fractional PDEs: A State of the Art



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Partial differential equations (PDE)s play an important role in the simulation of systems in applied sciences and technology. A lot of numerical methods have been developed for classes of PDEs arising in biology and medicine. Additionnally to the classical numerical techniques, other computational approaches also exist. Fractional calculus (FC) has been playing a crucial role in various fields of applied sciences and technology. It has some potential to change the model approach and control the results in order to tune with the realistic data. Beside its impact on problems with anomalous behavior, it was observed that FC can provide e cient numerical models having better consistencies with known data. The objective of the talk is to give a brief state of the art on existing numerical methods using a simple model problem for a PDE with integer and/or fractional orders. A swift review of some existing related works is also provided.

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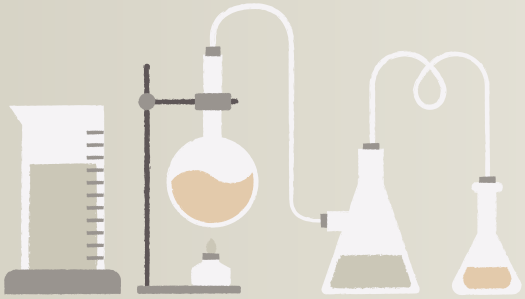
Raman-based imaging techniques: recent advancements and applications



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Raman micro-spectroscopy is a powerful, non-invasive, chemically selective and label-free imaging technique that derives its imaging contrast from chemical vibrations. Raman-based techniques emerged as significant characterisation tools for chemical analysis, materials science, biomedical and bio-sensing, etc… and continue to prove their usefulness as process analytical technologies (PAT) tools for bio-pharmaceutical research and manufacturing. Despite its numerous advantages, Raman microscopy suffers from the drawback of diffraction-limited spatial resolution, which restricts its ability to analyse changes and material behaviour at the nanoscale – an essential aspect in nanoscience and the design and development of novel nanodevices.

This talk will focus on the development of advanced modalities and techniques to enhance the capabilities of Raman microscopy and address its limitations, such as spatial resolution, signal-to-noise ratio, and imaging speed, offering thus promising avenues for technological advancements in nano-photonics, optoelectronics, bio-nanotechnology and material sciences.



CHEMISTRY

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Phenolic Acids, Flavonoids, and Antioxidant Properties of an Algerian Medicinal Astragalus Plant

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This work is devoted to the phytochemical and biological study of a medicinal plant belonging to the Algerian flora astragalus genus. This research was conducted to assess the phytochemical composition of methanolic extract using LCESIMS:MS ,following by testing in vitro antioxidant ability using DPPH and ß-caroten assays.

The liquid chromatography results showed that methanolicextract identified the presence of sixteen bioactive compoundsof the type phenolic acids and flavonoids.Rutin detected asmajor flavonoid with a concentration 6388.6090 mg/ml. Andshikimic acid was detected as major phenolic acid with aconcentration 325.9176 mg/ml.Moreover the result of totalcontent of polyphenols and flavonoids 175.83±1.95 µgGAE/mg extract and 43.10±0.27 µg EQ/mg extractrespectively.concerning antioxidant activity the methanolicextract has a good activity in all tests used with IC50 of DPPH ,ß-caroten tests IC50=3.74±1,04 µg/ml and 4.64±0.62µg/mlrespectively.Indeed , the presence of phenolic compounds maycontribute to their antioxidant activity.

Keywords: Astragalus, Phenolic acids, Flavonoids, Antioxidantactivity.

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Chemical composition of the essential of *Thymus ciliatus* (Desf).

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The Lamiaceae or Labiatae are a family of flowering plants with a cosmopolitan distribution containing about 236 genera and has been stated to contain 6900–7200 species [1]. In Algerian flora, there are 12 Thymus species from which 9 are endemic [2], among which Thymus ciliatus (Desf.) Benth, which is an endemic species from North Africa. Many Thymus species are used in various regions of the world in the treatment of bronchial, pulmonary, digestive and urinary infections and possess spasmolytic, antitussive and expectorant properties [3].

The essential oil of the aerial parts of *Thymus ciliatus* (Desf) belonging to the Lamiaceae family, was obtained by steam distillation and analyzed by GC-FID and GC-MS. 75 components were identified corresponding to 95.27% of the total oil. The major constituents of the oil were elemol (6.80%), carvacrol (5.86%), γ-muurolene (5.18%), β-sesquiphellandrene (5.09%), bicyclogermacrene (5.04%) , β-Pinene (4.49%) and curcumene (4.20%) together with other compounds at relatively low levels: 1,8 -cineol (3.66%), β-eudesmol (2.92%), β-bisabolene (2.81%), β-silinene (2.75%), camphor (2.64%),germacrone (2.34%), α-zingiberene(2.12%), δ-cadinene (2.08%).

It is interesting to notice that the chemical composition of the present essential oil differs from those reported in the literature. Our chemotype is exclusively characterized by high level of elemol, γ-muurolene β-sesquiphellandrene and bicyclogermacrene which have not been found in any reported essential oil of *T. ciliates.*

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A DFT STUDY OF THE MECHANISM AND REGIOSELECTIVITY OF 3+2 CYCLOADDITION REACTION OF 2-(2-OXOINDOLINE-3-YLIDENE)ACETATES WITH NITRONE.

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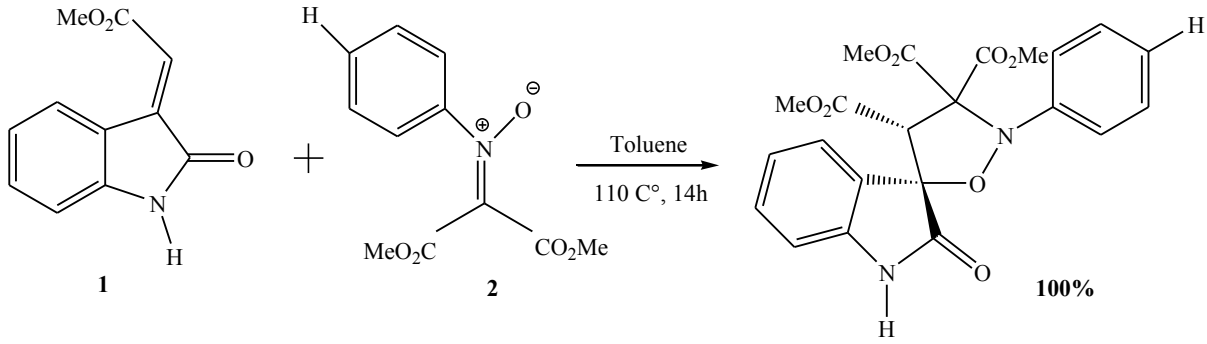
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In recent years, spiroheterocyclic scaffolds have attracted increased interest in the search for promising candidates for the development of new medicines; it is known that spiro derivatives of indolin-2-one are privileged structures in medicinal chemistry; due to their wide range of biological properties [1].

An interesting case of a 32CA reaction involving 2-(2-oxoindoline-3-ylidene) acetates **1** and ketonitrone **2** was described recently by Dmitriy et al. [2]. The cycloaddition was carried out in toluene at 110ºC and proceeded to obtain only 5-spiro regioisomers in good-to-high yields.

To confirm the experimental results and elucidate the origins of selectivity and the mechanistic nature of this cycloaddition reaction, we have conducted a computational investigation utilizing density functional theory (DFT) at B3LYP/6-31G(d,p) theoretical level.



Scheme 1: 32CA between 2-(2-oxoindoline-3-ylidene)acetate **1** and ketonitrone **2**.

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Chemical profiling and Anti-AGE properties of extracts from from algerian medicinal plants

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In a large project on Algerian plants, we are interested in their phytochemistry and biological properties. Particularly, in diabetes, a chronic hyperglycaemia occurs which is responsible for complications of diabetes through advanced glycation end-products (AGEs) formation.[1] SONAS lab developed an automated HTS assay, suitable for extracts, to evaluate their anti-AGEs potential.[2] This assay was used to screen different parts of 20 Algerian plants belonging to various families. Pressurized liquid extraction (PLE) led to 82 DCM and MeOH extracts. Seven were selected for their anti-AGEs properties and subjected to dereplication using LC-DAD-MSn. Some of them were selected for a bioguided fractionation.

Keywords: advanced glycation end-products (AGEs)

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The proposed methods were applied for the simultaneous determination of magnesium in real matrix samples. For this purpose, three real samples were analyzed commercial multivitamin (Additiva, manufactured by Dr. Scheffler, Germany), physiological serum (Saidal Pharm. Ind., Algeria) and drinking water (from commercial drinking water manufactured by IFRI, Algeria). The results of the prediction obtained by the present methods are summarized in Table 1 and compared with those obtained by atomic absorption spectrometry (reference method). These results show that PCR derivative model is able to predict magnesium in these samples with better precision than the PCR conventional one.

Table 1. Assay results for pharmaceutical preparations and drinking water.

Reported (AAS)		**PCR**		**PCR**	
		Original data		**First-derivative data**	
Samples	Found (µg/ml) **Mg(II)**	**Found (µg/ml) Mg(II)**	**Recovery (%)**	**Found (µg/ml) Mg(II)**	**Recovery (%)**
Multivitamins	**0.75**	**0.83**	**110**	**0.74**	**98**
Human serum	**3.065**	**3.12**	**101**	**3.09**	**101**
Drinking water	**0.63**	**0.56**	**89**	**0.64**	**103**
	RSD (%)	**2.05**		**1,87**	

AAS; atomic absorption spectrophotometry; RSD: relative standard deviation; the values were means of five replicate.

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Photocatalytic Removal of an Anionic Dye Using Hetaerolite Spinel under Solar Irradiation

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Water pollution, particularly from textile and plastic dye waste, poses a significant threat to aquatic ecosystems and human health. Anionic dyes, in particular, are highly soluble, stable, and resistant to degradation [1], making them difficult to remove using traditional wastewater treatment methods like activated sludge or coagulation-flocculation. As a result, these dyes can accumulate in water systems and disrupt aquatic ecosystems. Photocatalysis, which uses semiconductor materials to accelerate chemical reactions driven by light energy, has emerged as a promising solution to this problem [2]. By breaking down pollutants into less harmful substances like carbon dioxide and water [3], photocatalysis offers a sustainable and effective approach to reducing water pollution and protecting human health.

This study investigates the degradation of Congo Red (CR), an anionic dye, using $ZnMn_2O_4$ nanoparticles under solar light. The nanoparticles were synthesized via the sol-gel auto-combustion method and characterized using various techniques to assess their structural, physical, and electrochemical properties. XRD confirmed the tetragonal spinel phase with minor ZnO presence. $ZnMn_2O_4$ exhibited a direct optical band gap of 1.97 eV, and its p-type behavior was confirmed via a Mott-Schottky plot, indicating a flat band potential of -0.125 V/SCE. CR adsorption followed the Langmuir isotherm model. Photolysis tests confirmed CR's stability under solar irradiation, with $ZnMn_2O_4$ achieving 87 % degradation efficiency after 3 h, following pseudo-first-order kinetics. Critical factors such as dye concentration, photocatalyst dose, and pH significantly affected the degradation process, emphasizing the importance of optimizing these parameters for efficient photocatalytic degradation of CR. XRD

analysis before and after photocatalysis revealed nearly identical peak positions, confirming the material's stability.

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DFT investigation of copper(I) in linear XCuL' and $(LCuL')^+$ (X = Cl, CH_3, CN, CF_3, L = CO, NH_3, PH_3 and L' = C_2H_2, C_2H_4, C_4H_6, C_6H_6 and NHC) complexes: Electronic structures and nature bonding from energy decomposition analysis2024

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This DFT (Density functional theory) investigation using BP86 and B3LYP functionals and TZP basis set is dealing with the bonding, the electronic structure and the interaction types occurred within the XCuL' and $(LCuL')^+$ (X = Cl, CH_3, CN, CF_3, L = CO, NH_3, PH_3 and L' = C_2H_2, C_2H_4, C_4H_6, C_6H_6 and NHC) complexes.

The optimized structures and energy decomposition analysis of XCuL' and $(LCuL')^+$ complexes were employed to provide a relationship between the bond lengths, the X-Cu-L' and L-Cu-L' bond angles, the Wiberg indices, the Mayer bond orders, interaction energies and the Cu-L' bonding character. The energy decomposition analysis indicates that the interactions occurred for various L' ligands are more electrostatically than covalently bonded to the Cu(I) [1-3] center formally of +I oxidation state. The different contributions stemming from electrostatic and orbital interactions are significant, in relationship with the ionic and covalent characters, respectively. The contribution from σ-donation to the bonding energy was found more important for the NHC ligand than the alkene and alkynes ones, where the two later contribute equally in their interactions with the metallic fragment. However, the contribution from the π-back-donation was found to be comparable for all complexes. The σ-bonding contributes more than 50% into the total orbital interaction overtaking those of π type, in accordance with the population of the copper 4s orbital, particularly in the presence of C_6H_6 and NHC ligands. Besides, it has been shown that the ΔE_{prep} contributes weakly in the deformation of the interacting fragments as well as the BSSE correction which impacts weakly or negligibly the interactions between the fragments composing different XCuL' and $(LCuL')^+$ complexes.

Keywords: σ-donation, π-backdonation, mixed copper electronic configuration, NBO analysis.

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In Silico Study of a Heterocyclic Derivative on Anticancer and Anti-Alzheimer's Effects

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Heterocyclic compounds exhibit significant biological activity and play a crucial role in the treatment of various diseases, including diabetes, Alzheimer's, and cancer. Developing medications that target multiple diseases is essential and could help reduce the number of drugs required in the future.

The aim of this study is to demonstrate the anti-cancer and anti-Alzheimer's activity of 3-(benzofuran-3-yl)-5,7-diphenylpyrazolo[1,2-a][1,2,4]triazol-1(7H)-one through docking design. Additionally, the pharmacokinetic (ADMET) properties of the compound will be assessed to evaluate its potential for medicinal applications and therapeutic efficacy.

This research provides evidence that the molecule is a strong inhibitor of acetylcholinesterase [1], cyclooxygenase [2], and tubulin [3], making it a bioactive compound with substantial medicinal potential in the treatment of cancer and Alzheimer's. The findings suggest that such compounds could play a crucial role in drug development, offering new avenues for medical research and clinical applications.

Keyword
docking design, anti-cancer, anti-Alzheimer's, acetylcholinesterase, cyclooxygenase, tubulin, ADMET

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La composition chimique des huiles essentielles de l'espèce *Paronychia nivea* d'Aurès (Algérie)

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Résumé

Le genre *Paronychia* appartient à la famille des Caryophyllacées. Il est représenté par cinq espèces dans la flore d'Algérie. *Paronychia nivea* L. est une plante vivace connue sous le nom de (Kessarat lahdjer) [1]. L'infusion des parties aériennes de la plante est utilisée dans la médecine populaire espagnole pour purifier le sang, réguler la circulation et traiter la goutte, ainsi que comme agent contre les dermatites et comme expectorant [2]. Il est également utilisé comme cholagogue, dermatologique, anti-infectieux, lithotritique, diurétique, digestif et antihypertenseur [3].

Notre travail consiste à évaluer la composition chimique de l'huile essentielle de lentisque extraite de ses parties aériennes. Plusieurs paramètres ont été considérés à savoir : la période de récolte et la partie aérienne de la plante utilisée. Les échantillons de la plante sont récoltés au printemps à Merouana dans la wilaya de Batna. L'huile essentielle est extraite par hydrodistillation à partir des parties aériennes. La composition chimique des huiles extraites a été effectuée par l'analyse CG-SM.

Les résultats de cette analyse révèlent la présence notamment de monoterpènes et de sesquiterpènes hydrocarbonés. En conclusion, ces résultats remarquables nous incitent à compléter l'étude biologique des huiles essentielles extraire de cette plante et en évaluera leur importance biologique.

Mots clé : *Paronychia*, Caryophyllaceae, hydrodistillation, huiles essentielles, CG-SM ; composition chimique.

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Etude the depollution of aqueous effluent by coupling electrodialysis to electrochemical oxidation

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Abstract

The presence of organic materials in industrial waste can constitute a serious threat to the environment when they are released without prior treatment into the biosphere. The malfunction and corrosion of industrial installations can also generate other pollution (metallic, organometallic and especially organic) which has harmful effects on aquatic flora and fauna, but also on human and animal populations which consume untreated water. Treatment will therefore be essential to degrade these materials which are harmful to the environment. The coupling of the anodic oxidation process with electrodialysis, which presents itself as a new, rapidly expanding technique with a wide variety of applications, arouses special interest for the treatment of industrial effluents containing a range of toxic contaminants. In this work, the target pollutant is dodecyl benzene sulfonate (SDBS).The study consists of optimizing the parameters which have an influence on degradation. After optimization of the coupling parameters, the degradation efficiency obtained from SDBS is 98.43% for a contact time of 120 minutes, oxidation density 40 $mA.cm^{-2}$, electrodialysis current density is 20 $mA.\ cm^{-2}$, Na_2SO_4 at 0.1 N used as supporting electrolyte and a natural pH.

Keywords: Electrodialysis, Electro- oxidation, Process coupling, Dodecyl benzene sulphonate, Degradation of SDBS, pollution of water.

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Synthesis, Molecular structure, Hirshfeld surface analysis and DFT calculations of some quinoline hybrids

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Abstract:

During the last two decades, quinoline and its derivatives have attracted more attention from organic chemists due to their considerable biological and pharmacological activities.[1-3] On the other hand, piperidine (hexahydroazine) and morpholine (tetrahydro-1,4-oxazine) are two important heterocyclic structures widely used in organic chemistry as solvents, catalysts, and building blocks in many synthetic protocols. Moreover, piperidine is asserted as the most encountered heterocycle in pharmaceuticals [4,5], while the morpholine ring is present in the structure of many drugs used in various therapeutic areas. [6,7]

In continuation and development of our work on the synthesis and biological evaluation of original quinoline-based compounds [8-10], we report here a comparative study concerning a quinolone/morpholine and a quinolone/piperidine hybrids; and their precursor 3-(2-Chloroquinolin-3-yl) oxirane-2,2-dicarbonitrile. The study involves spectroscopic characterization, experimental analysis by X-ray diffraction and DFT calculations using the B3LYP functional and 6–311G(d,p) as the basis set. The theoretical results are in good agreement with the experimental data. In addition, 2D and 3D Hirshfeld surfaces analysis were used to determine intermolecular interactions in the crystal network.

Keywords: Quinoline, Hybrid compound, Single crystal, Hirshfeld surface, DFT.

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Mononuclear nickel complex: synthesis, spectroscopy and electrochemical study

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The Schiff bases of 4-aminoantipyrine and its complexes have variety of applications in the biological, clinical and pharmacological fields [1]. It is known that some drugs showed increased activity when administered as metal chelates rather than as organic compounds. The coordinating property of 4-aminoantipyrine can be modified into a flexible ligand system by condensation with a variety of reagents like aldehydes, ketones, thiosemicarbazides, carbazides etc. [2,3]. For a long time bidentate Schiff base complexes have attracted many interests in the field of coordination chemistry [4].

Here in, we report the synthesis of a new Schiff base ligand, was prepared by reaction of 4-aminiantipyrine with 2,5-dihydroxybenzlaldehyde and its corresponding nickel complex. High purity, good Yield for the resulting products and the molar conductance data revealed that the ligand and the metal complex is a non-electrolyte nature (4.9/ 6.8 Ω^{-1} $mole^{-1}$ cm^2 for L and NiL resp). The spectroscopic analysis using FTIR, UV-Vis, (^1H -^{13}C) NMR confirmed the structure of newly obtained materials.

Electrochemical behaviour for both the ligand and the corresponding complex have been observed by cyclic voltammetry (CV) at room temperature with a glassy carbon (GC) working electrode in DMF/10^{-1}M TEAP under nitrogen atmosphere. The complex gave a reversible cyclic voltammograms response in the potential range -1.8 à -1.2 V involving a single electron redox process Ni(II)/Ni(I).

Keywords: Nickel complex, Schiff base, 4-aminoantipyrine, cyclic voltammetry.

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Insights into the Free Radical Scavenging Mechanism of Daphnetin in Physiological Conditions: A DFT-Based Study

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Oxidative stress results from an imbalance between excess free radicals and antioxidants [1]. Free radicals, including ROS and RNS, are reactive molecules that play roles in cell signaling but can also damage cellular components when in excess, leading to diseases like cancer, diabetes, and neurodegeneration [2]. Antioxidant systems typically neutralize free radicals, but under certain conditions, they become ineffective, necessitating the intake of external antioxidants.

Daphnetin (7,8-hydroxycoumarin) is a bioactive polyphenol isolated from Daphne plants [3], with traditional use in China for treating bleeding disorder. It shows broad pharmacological activity, including antioxidant, anti-inflammatory, and anticancer effects [4]. Daphnetin inhibits enzymes like lipoxygenase and scavenges various radicals [5]. It is non-toxic, making it a promising drug candidate [6].

Despite extensive experimental research on daphnetin's antioxidant activity, its specific mechanism against radical species remains unexplored. No prior experimental or theoretical studies have addressed its reactivity towards ROS and RNS. Building on previous work [7, 8], this study investigates the mechanism and kinetics of DAP's reactions with ROS and RNS, including $HO^{\bullet}$, $HOO^{\bullet}$, $NO^{\bullet}$, and $NO_2^{\bullet}$, using quantum chemistry and computational kinetic methods in physiological environments.

As a result, daphnetin exhibited strong scavenging activity against $HO^{\bullet}$ radicals in physiological environments, and is predicted to also effectively scavenge $HOO^{\bullet}$ and $NO_2^{\bullet}$ radicals in water, with rate constants of 1.51×10^7 and 4.79×10^8 $M^{-1}s^{-1}$, respectively. The FHT mechanism governs the $HO^{\bullet}$ radical scavenging in lipid and aqueous media, while SPLET is the primary mechanism for $HOO^{\bullet}$ and $NO_2^{\bullet}$ radical scavenging in water. Theoretical predictions align well with experimental data, supporting the accuracy of the calculations.

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New cellular imaging contrast agents based on lanthanides (III) and a Tow-Connected Ligand

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Nine lanthanide-organic frameworks $[Ln_2(pda)^{3-}\ (H_2O)]\cdot 2H_2O$ [Ln = Ce(1), Nd(2), Sm(3), Gd(4), Tb(5), Dy(6), Tm(7), Yb(8) et Lu(9) ; H_2dpa = 1,4-phenylenediacetate], have been prepared by hydrothermal reactions of the corresponding lanthanide nitrates ($Ln(NO_3)_3$, xH_2O), and 1,4-phenylenediacetic acid. The complexes have been characterized by single-crystal, powder X-ray diffraction and IR spectroscopy. All the MOFs (LOFs) are isostructural and involve of unidimensional Ln–COO chain that are cross-linked by the $–CH_2C_6H_4CH_2–$ spacers of the $pda^{2–}$ anions in a tri-dimensional compressed honeycomb-shaped network with unidimensional open channels, which accommodate guest and coordinated water molecules. The metal centres are eight-coordinated to give polyhedral coordination geometries with an LnO_8 donor set. The fluorescence properties of complexes were investigated and give us a first view of their applications in medicine and biology's fields [1, 2].
Keywords: lanthanide-organic frameworks, crystal structure, X rays diffraction, fluorescence luminescent markers for cellular imagery, laser.

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Jijelian green carob (*Ceratonia siliqua* L.): Bioactive substances content, and antioxidant potential

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Carob (*Ceratonia siliqua* L.) is a perennial plant in the Fabaceae family native to the Mediterranean region [1], which is the principal carob production center with an annual production of more than 135,000 tons [2]. The carob tree, part of the Oleo-Ceratonion, is widely spread across Algeria, covering territories from east to west, at low and medium altitudes as well as in semi-arid and humid bioclimates [3].

The main purpose of this research was to assess the proximate composition and physicochemical properties of Jijelian wild green carob collected from three different lacalities (El Emir Abdelkader, Chekfa, and Texenna), as well as to investigate its antioxidant potency. In terms of bioactive molecules level, Texenna green pods had the highest levels of polyphenols, flavonoids, and flavonols. Furthermore, the total antioxidant capacity of the methanolic extracts determined using the phosphomolybdate method was found to be 154.62 µg AAE/mg DM. These promising findings revealed that unripe *Ceratonia siliqua* L. from the Texenna region is a rich source of natural antioxidants that might be used in a wider range of functional food compositions.

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In vitro photoprotection and antioxidant capacity of some Algerian *Centaurea* species

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Solar ultraviolet radiation (UVR) causes the most harm to biological compounds. UVC rays (100-280 nm) are extremely harmful to skin. Fortunately, molecular oxygen and ozone in the earth's troposphere mostly absorb it. UVB (290-320 nm) makes up only about 5% of terrestrial UVR, but its effects are typically far greater than those of UVA (320-400 nm). UVR's clinical effects on normal-appearing human skin are mostly aggressive, including erythema, pigmentation, suppression of acquired immunity, and enhancement of innate immunity, all of which are caused by UVB [1-3], and blood pressure reduction caused by UVA. Photocarcinogenesis and photoaging are both long-term effects [3-5]. A number of novel approaches have been proposed to improve sunscreens. It has been proposed that incorporating antioxidant phenolic extracts into sunscreens can enhance photoprotective properties and provide greater protection, thereby replenishing the skin's natural reservoirs [5].

Thus, the goals of this study are to ascertain the antioxidant activity of some *Centaurea* extracts from Algerian flora as well as to highlight their photoprotective effects.

The antioxidant capacity of the sample was determined by the phosphomolybdenum test, DPPH, and ABTS scavenging activities. Furthermore, the photoprotective activity was assessed by measuring the sun protection factor (SPF) using the dilution method. The results showed that polar *Centaurea* extracts have a rich level of polyphenols (phenolic and flavonoid contents). Among the tested extracts, ethyl acetate extracts exhibited the best antioxidant capacity as well as the highest value of SPF (superior to SPF 30).

Algerian *Centaurea* extracts may thus provide a natural antioxidant alternative for photoprotection and skin care.

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The influence of time on the biosynthesis of nanoparticles from medicinal plant extracts

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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 extract of a medicinal plant
"In our work, we study the biosynthesis of nanoparticles based on extracts from medicinal plants with respect to time (1h, 3h, 24h, 48h, 72h). We found that the formation of nanoparticles after 72 hours was more significant than at the other durations.
"Therefore, we can conclude that the formation of nanoparticles increases with time under the given operating conditions.

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Assessment of phytochemical content and Antioxidant activity of *Centaurea dimorpha* Viv. (Asteraceae) extracts

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Abstract

The present study aims to evaluate the antioxidant capacity and the phytochemical content of the ethyl acetate (EtOAc) and n-butanol (n-BuOH) extracts of the species *Centaurea dimorpha* Viv, an endemic species that belongs to Asteraceae family.

In this study total phenolic and flavonoid contents was determinate using Folin-Ciocateu and aluminum chloride methods, respectively. The antioxidant activity was measured through three *in vitro* methods, DPPH radical scavenging, phenanthroline and total antioxidant capacity (TAC) by phosphomolybdenum methods.

The highest levels of TPC and TFC were recorded by the ethyl-acetate extract (119.20± 0.32μg GAE mg^{-1}, 50.65±0.43μg QE mg^{-1}, respectively) compared to n-butanol extract (79.37±1.13μg GAE mg^{-1}, 28.24±0.30 μg QE mg^{-1}, respectively).

The EtOAc extract had a good DPPH radical scavenging effect (20.91±0.13 μg AAE mg^{-1}) compared to n-BuOH (19.05±0.45 μg AAE mg^{-1}). Total antioxidant capacity (TAC) of extracts was determined as 99.67±1.28 μg AAE mg^{-1} for EtOAc extract and 67.28±1.64 μg AAE mg^{-1} for n-BuOH extract, the results revealed that EtOAc extract was found to be more effective compared to n-BuOH extract. By the phenanthroline method, the best result was obtained with EtOAc extract (152.63±0.49 μg AAE mg^{-1}) followed by n-BuOH extract (57.19±4.72 μg AAE mg^{-1}). It is clearly shown that there is good correlation between DPPH, Phenanthroline and TAC methods, which implies that the antioxidants in this plant were able to scavenge free radicals and reduce oxidants where we find ethyl acetate extract possessed high radical scavenging activity and oxidant reducing activity compared to n-butanol extract.

The results obtained show the possibility to use ethyl acetate extract as a natural antioxidant agent in several anti-aging formulation.

Keywords: antioxidant activity, DPPH, TAC, Phenanthroline assay, *Centaurea dimorpha*.

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Photoprotective activity of plant ethanolic extract

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It is well recognized that phenolic compounds have biological properties that support skin care. *Teucrium polium* is a perennial wild flowering plant that is highly prominent in a number of traditional use.

To assess the photoprotective power of ethanolic extract of *Teucrium polium*, its sun protection factor (SPF) was determined. After dissolution of the extract with ethanol, SPF is determined by measuring absorption in the 290-320 nm range at 5 nm difference, followed by application of the Mansur equation.

The *Teucrium polium* extract absorbs UV radiation and is classified in the 'High protection' category with an SPF of 38,62. High phenolic content exhibit substantial SPF values and effective UV protection**.**

The ethanolic extract of *Teucrium polium* can be formulated as a natural sun screen.

Keywords: photoprotective, *Teucrium polium,* ethanolic extract, Mansur equation

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New Green Synthesis of 1-amidoalkyl-2- naphthol

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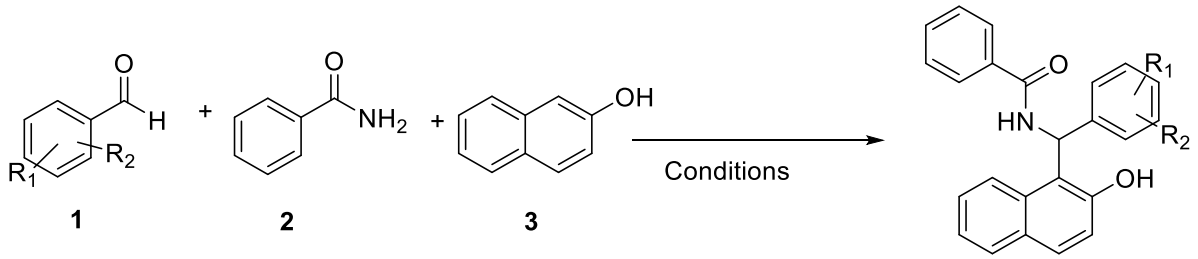
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Multicomponent reactions (MCRs) play an important role in green synthesis, helping researchers prepare compounds in a short time, using eco-friendly procedures and obtaining high yields. 1-amidoalkyl-2-naphthol are synthesized via Betti reaction using various approaches and many catalysts (Mushtaq et al., 2023). Betti bases represent a broad spectrum of applications in medicinal chemistry. They show potent biological activities including antibacterial (Bananezhad, Islami & Khabazzadeh., 2019), antioxidant (Boudebbous et al., 2020), and anticancer activities (Puerta et al., 2019).

This work is devoted for the synthesis of 1-amidoalkyl-2- naphthols via Betti reaction. The reaction was performed in the presence of 1eq of an aromatic aldehyde, 1eq of a 2-naphthol and 1.2eq of a benzamide, under green conditions (Scheme 1). A series of the target compounds were prepared using various aldehydes. The synthesized derivatives showed moderate to good yields. The structures were identified by the spectroscopic methods 1H NMR, 13C NMR and IR.



Scheme.1: Synthesis of 1-amidoalkyl-2- naphthol

Keywords: Green Synthesis, Betti reaction, 1-amidoalkyl-2- naphthols.

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Isolation and identification of Sterols from *Echium italicum L. species*

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Echium italicum L., also known as Italian viper's bugloss, is a plant belonging to the genus *Echium L.* within the family Boraginaceae. The Boraginaceae family, known as the borage or forget-me-not family, includes around 150 genera and 2,000 species [1]. The genus Echium, with about 70 species, is native to North Africa, Europe, Central Asia, and the Macaronesian islands. These plants are valued for their medicinal properties and high content of beneficial fatty acids. They have been traditionally used for treating various ailments and their seeds are sought after for cosmetic and skin-care applications. Some Echium species are invasive in places like Australia [2-3].

This study aims to investigate the phytochemical profile of the E. italicum species and identify the compounds it contains. Phytochemical screening of various extracts (PE, AcOEt, n-Butanol) from the entire plant reveals the presence of alkaloids, sterols, flavonoids, and tannins. Using chromatographic methods, the chemical analysis of the ethyl acetate extract identified two sterols: β-sitosterol and β-sitosterol-3-O-glucopyranosyl.

Keywords: Boraginaceae, *Echium italicum*, phytochemical screening, sterols.

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HPLC Analysis of a Plant from the Genus Vicia (FABACEAE)

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Abstract

Fabaceae is one of the largest families of flowering plants in the world, with approximately 730 genera and over 19,400 species according to the Royal Botanic Garden, Edinburgh (2010). This family is known for its extensive use in traditional medicine, and recent phytochemical studies have highlighted the wealth of secondary metabolites in these plants, such as polyphenols. and its remarkable biological activity like antioxidant activity. [1]

The genus Vicia is one of the important genera within the Fabaceae family. In Algeria, the genus Vicia is represented by 83 species [2] . Recent studies on plants from this genus have demonstrated the presence of various secondary metabolites, including polyphenols, flavonoids, and saponins. [3]

Phytochemical screening of the hydroalcoholic extract from the aerial parts of the species, conducted using various qualitative tests, revealed that the plant is very rich in secondary metabolites, particularly flavonoids and saponins. Total contents of polyphenols and flavonoids were determined.

We also studied the chemical composition of the hydroalcoholic extract of the plant using HPLC, and the results led us to conclude that the extract is rich in simple phenolic acids.

Keywords: Fabaceae, Vicia, polyphenols, HPLC, phenolic acids.

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Effect of a new green catalyst on aspirin synthesis

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Abstract

Currently, acid catalysts are widely used in various organic synthesis processes to facilitate chemical reactions, accelerate reaction times, and increase yields [1,2]. However, the use of these acid catalysts can also present significant drawbacks [3,4].

Our project aims to promote an innovative natural catalyst: banana peel ash, for the preparation of aspirin; one of the esters that has generated significant interest in scientific research for its advantageous biological properties.

The study also relates to the effects of some parameters on the yield and kinetics of the reaction, the effects of catalyst amount, temperature and catalyst regeneration.

According to the obtained results, banana peel ash has been demonstrated to be an extremely effective natural catalyst for the synthesis of aspirin. This discovery paves the way for using this natural catalyst in the production of a variety of organic molecules, marking a promising turning point in the field of green chemistry through waste valorization. Noteworthy aspects of this protocol include high yields, short reaction times, catalyst recyclability, and simple product isolation.

Keywords: Banana peel; Heterogeneous catalyst; Aspirine

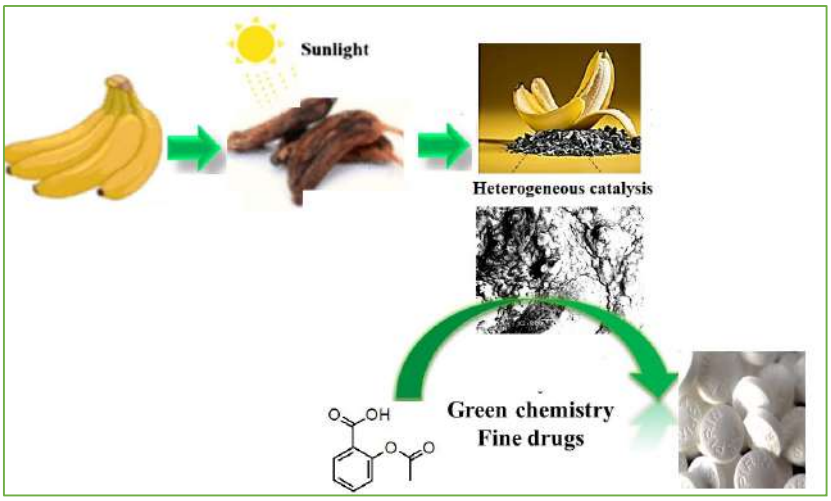
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Graphical abstract

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2D numerical simulation of nitrogen oxide conversion in a wire-cylinder reactor subjected to non-equilibrium

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In recent years, the global industrial development has resulted in increased energy consumption, which has caused of the atmospheric disturbance and the augmentation in certain gaseous pollutants such as nitrogen oxides NOx [1]. In this paper, we proposed to numerically simulate the evolution of the density of these nitrogen oxides NO, NO_2 and NO_3 present in the gaseous mixture N_2/O_2[2,3], which is subject to different values of the reduced electric field: 50, 100 and 150 Td (1Td = 10^{-17} V.cm^2). The simulation is carried out in the wire-cylinder reactor with a length of 10 cm and a radius of 12 mm, for 2 ms. The model takes into account twelve different chemical species reacting following fifty selected chemical reactions. The obtained results clearly show the impact of the reduced electric field on the conversion of nitrogen oxides.

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Silver Nanoparticles and Environmental Sustainability: Advances, Challenges, and Future Directions

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In this study, the catalytic capacity of eco-synthesized silver nanoparticles (AgNPs) is examined for the degradation of methylene blue, a hazardous environmental contaminant present in water [1]. The AgNPs were prepared under ambient conditions using the antioxidant content of the extract of Lawsonia inermis (henna), and their bioreduction capacity was studied in detail [2]. This process is entirely eco-friendly, with no toxic and hazardous solvents [3]. The biosynthesized AgNPs were nanoscale, and their morphology, size, and optical properties were characterized using field emission scanning electron microscopy (FE-SEM), thermogravimetric analysis, energy dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), and ultraviolet-visible spectroscopy (UV-Vis). The biosynthesized AgNPs proved to be active catalysts, particularly in the presence of reducing agents such as sodium borohydride, for the degradation of toxic organic dyes such as methylene blue (MB) in contaminated water. The AgNPs are stable and reusable to reduce MB to its leuco form in an aqueous medium in the absence of reducing agents.
Key words: Green synthesis, silver nanoparticles, Extraction, Degradation, Catalytic activity.

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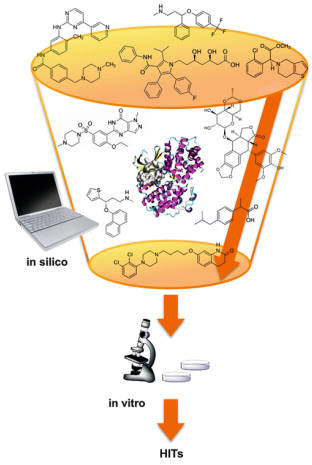
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In-silico design and computational chemistry for drug discovery. Current and future perspectives!

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The process of drug discovery and development is challenging, time-consuming (> 10 years) and expensive (> one Billion $). Computational chemistry based on in-silico methods and Computer-Aided Drug Design (CADD) techniques (Figure) can substantially widen this long process search by providing tools able to predict the best drug-target binding affinities and rationalize the process by reducing duration, cost, and attrition rate [1]. Furthermore, recent advances in computer hardware and software, such as the analysis of cellular 3D images and the development of novel routes for synthesizing bioactive molecules, have significantly impacted drug discovery [2].

Today in-silico methods have become an effective and indispensable tool in therapeutic development and advancing pharmaceutical research. Although nature has been the most important source of medicinal agents, nowadays, most therapeutic agents with potent drug activity are synthetic small organic molecules (heterocyclic) that can activate or inhibit the function of a biomolecule, generally a protein, which in turn results in a therapeutic or prophylactic benefit to the patient.

Here we present an overview of computational and in-silico methods used in different facets of drug design and highlight some recent successes. For this purpose, both structure-based and ligand-based drug discovery methods [3] are discussed, including quantitative structure-activity relationship (QSAR) advances, protein-ligand molecular docking, dynamics simulations, and ADMET properties for oral bioavailability.

To support this review, anticancer activity was in-silico assessed with an emphasis on novel bioactive molecules featuring potent cancer inhibition, which are highlighted [4]. Nowadays, in-silico techniques play an ever-increasing role in drug discovery and are critical in the cost-effective identification of promising e.g., cancer inhibition drug candidates from the hits to the leads.

Keywords: Bioactivity, in-silico, CADD, Virtual Screening, Anticancer Inhibition, QSAR, Molecular & Dynamics Docking, ADMET.

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Molecular Simulation of Encapsulating Polycyclic Aromatic Hydrocarbons (PAHs) for Environmental Safeguarding

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This research addresses the urgent environmental and health risks posed by Benzo[a]pyrene (BaP), a highly toxic and carcinogenic polycyclic aromatic hydrocarbon (PAH) commonly released into the environment through industrial activities. As BaP accumulates in ecosystems, it threatens wildlife and poses serious health risks to humans, including cancer and respiratory issues.

To tackle this challenge, the study employs advanced quantum methods, such as the PM7 semi-empirical approach and DFT D3 (B3LYP D3) dispersion corrections, to explore the encapsulation potential of various macrocyclic compounds. The focus is on innovative materials like cyclodextrins, pillararenes, and cucurbiturils. Among these, cyclodextrins—particularly β-cyclodextrin—stand out due to their exceptional stability and high complexation energies.

These findings not only enhance our understanding of BaP encapsulation but also pave the way for developing effective strategies to detect and eliminate this hazardous compound from contaminated sites. By leveraging these materials, we can make significant strides toward protecting our environment and public health from the harmful effects of PAHs in industrial areas.

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The First International Congress on Recent Advances in Mathematical, Physical and Chemical Sciences (1st-ICRAMPCS 2024)
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ABSTRACT

To assess the risks to human health caused by exposure to PM10 and associated trace elements, a measurement campaign was carried out at the Faculty of Earth Sciences in Constantine, 64 samples were collected over a period ranging from January 2015 to February 2016, the trace elements Pb, Cr, Co, Ni, Zn, As, Cd, V and Mn were analyzed by Mass Spectrometry (ICP-MS).

The results reveal an annual average PM10 concentration of around 55.7 µg/m^3 was three times higher than the guideline value recommended by the WHO (20 µg/m3). The average concentrations of Pb, As, Cd and Ni were 79.43, 0.46, 0.22 and 1.24 ng / m^3, was lower than the European limit values (set at 500, 6, 5 and 20 ng / m^3 respectively).

The risk levels of exposure (R) to carcinogenic heavy metals were in the following order: Cr>As>Cd>Co>Ni. Furthermore, these carcinogenic elements represented the greatest cancer risk in adults compared to children, chromium (Cr) cancer risks exceeded the threshold of 10-6, which could result in a cancer risk to human health since any cancer risk below the threshold value of 10^{-6} is considered negligible by the US EPA [1].

The sum of the risk levels (HI) for the nine heavy metals were 0.19 for children and 0.42 for adults, greater than 0.1 but less than 1. This suggests that the non-carcinogenic effects of heavy metals on PM10 are unlikely. Generally speaking, the impact on human health through inhalation of the trace elements analyzed appears to be rather low.

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Computational Evaluation of Bioactive Fabaceae Metabolites: ADME-Tox Profiling of Cirsiliol, Carnosol, and Luteolin for Therapeutic Potential

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This study explores a species from the Fabaceae family native to the Jijel region, known for its rich diversity of approximately 240 genera and over 7,000 species [1,2]. Research on these plants has revealed various secondary metabolites, including saponins, triterpenes, and flavonoids, which possess significant biological activities. These compounds are important in the pharmaceutical industry for their roles as natural sweeteners and therapeutic agents, exhibiting properties such as hepatoprotective, antibiotic, UV-protective, anti-inflammatory, antitumor, antiallergic, and anti-ophthalmic effects [3, 4].

Furthermore, in silico drug design has revolutionized drug discovery by facilitating the early prediction of ADME-Tox (absorption, distribution, metabolism, excretion, and toxicity) profiles [5, 6]. This study conducts a comprehensive computational analysis of cirsiliol, carnosol, and luteolin, focusing on their ADME-Tox characteristics. Techniques like molecular docking and Density Functional Theory (DFT) are utilized to assess drug-likeness, bioavailability, and potential toxicity risks. The findings indicate that these compounds exhibit favorable ADME profiles, showing high gastrointestinal absorption and minimal toxicity risks, thus emphasizing their therapeutic potential for future experimental validation in preclinical studies.

Keyword: Fabaceae, secondary metabolites, DFT, ADME-Tox.

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Analyzing Fatty Acid Composition in Algerian Rapeseed Oil: Nutritional Benefits and Economic Implications for Crop Diversification

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Rapeseed represents a significant opportunity for Algerian agriculture, both economically and for crop diversification. Based on the chromatograms of fatty acid methyl esters, we determined the fatty acid composition of the lipid extracts (simple lipids, neutral lipids, and total lipids) from rapeseed [1-2].

The oil extracted from rapeseed across all fractions provides a nutritional bridge. The fatty acid composition of rapeseed from the Bordj Bou Arreridj region indicates that the vegetable oil from these seeds is of good quality, rich in essential fatty acids crucial to the human body, such as linoleic and oleic acids, which account for over 60% and 15%, respectively. These fatty acids help maintain cholesterol levels and reduce the risk of cardiovascular disease.

This fatty acid composition allows us to classify rapeseed oil among linoleic-type vegetable oils.

Rapeseed oil also contains a significant amount of saturated fatty acids (palmitic acid: 4.32-5.16%).

Keywords: rapeseed, lipids, fatty acids, GC chromatography

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Degradation of rhodamine B by the Fenton process

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Water covers about 72% of the Earth's surface, with 97.2% of it being saline and only 2.8% fresh water. Consequently, fresh water reserves directly usable by humans account for only 0.65% of the planet's total water mass [1]. Water is extensively used in industrial environments for various applications [2]. For example, the textile industry is responsible for effluents containing toxic, non-biodegradable dyes. Treating this wastewater has become a major global issue, underscoring the need for more efficient and cost-effective methods to degrade organic dyes in wastewater [2].

Advanced Oxidation Processes (AOPs), developed in recent years, are drawing significant attention for their ability to effectively break down most organic pollutants. They work by producing free radicals as the primary active substance for the complete removal of organic pollutants, including dyes [3].

In this study, we focused on the degradation of Rhodamine B dye using the Fenton process, with potassium persulfate activated by iron (II) as an oxidant. The degradation of Rhodamine B was carried out by varying the concentrations of potassium persulfate (PS) as the oxidant and iron (II) as the catalyst. Complete degradation of a 10 µM Rhodamine B solution was achieved within two minutes at 25°C, under stirring, with an iron/PS concentration ratio of 0.5.

Keywords: Fenton process, Rhodamine B, Advanced Oxidation Processes

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Advancements in Nanocomposite Materials for Effective Water Decontamination

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abstract

Nano size material displays exceptional electrical, magnetic, optical, catalytic and medical characteristics relative to the conventional and commercially available bulk materials**[1]**. These properties are as a result of its quantum confinement effects, as well as large surface area per unit volume**,**NiO nanoparticles are of great use as a result of its uncomplex nature of its synthesis and important talented physical and chemical characteristics**[2]**. NiO NPs have been synthesized by several procedures including chemical bath deposition , sol–gel procedure , thermal evaporation , pulsed laser deposition , hydrothermal , green method , and spin coating**[3]** .
in this study the catalytic ability of green synthesized nickel oxide nanoparticles (NiO NPs) is investigated for degradation of methylene blue as a hazardous environmentally contamination in water. The NiO NPs was prepared at ambient conditions using the antioxidant content of Lawsonia inermis **[4]**. The biosynthesized NiO NPs were systematically characterized through FT-IR spectroscopy, scanning electron microscopy (SEM)coupled with energy-dispersive X-ray spectroscopy (EDX), and X-ray diffraction (XRD),thermogravimetric analysis (TGA), Zetasizer Nano and zeta potential,. The biosynthesized NiO NPs were found to be active catalysts, particularly with the reducing agents for instance sodium borohydride, for the degradation of the toxic organic dyes such as methyl orange (MO) and methylene blue(BM) in contaminated water.The influence of different parameters such as temperature, mass, and contact time were studied. The study of the kinetics as a function of concentration showed that the percentage removal of methylene blue increases as the mass of the catalyst increases. The values of ΔG° and ΔH° show that the degradation process studied is spontaneous and endothermic.

Keywords: degradation, depollution, sodium borohydride, methylene blue, nickel

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Design, synthesis, biological evaluation and molecular docking Studies of novel pyrazolone derivatives as anticancer agents

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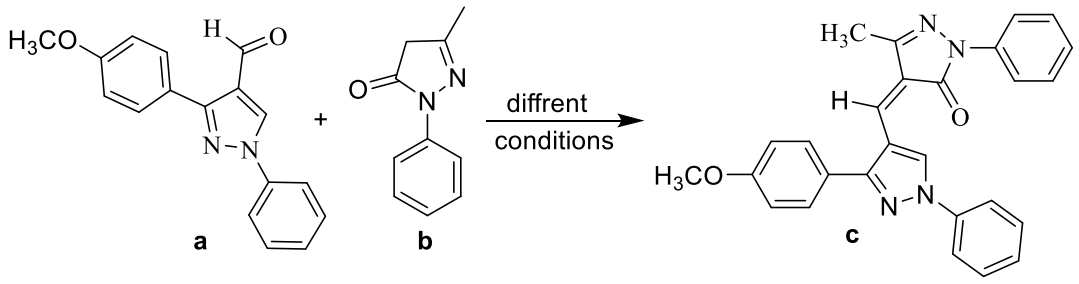
Knoevenagel condensation is one of the most important methodologies for carbon-carbon double bond formation in synthetic organic chemistry, in which α,β-unsaturated products formed via a nucleophilic addition reaction between active methylene and carbonyl compounds followed by a dehydration reaction.[1,2]

Pyrazolone chemistry has become highly significant owing to its wide-ranging applications in the pharmaceutical industry.[3,4] Currently, Numerous FDA-approved drugs featuring the pyrazolone nucleus have been researched and developed. for example, metamizole has been utilized in the treatment of perioperative pain, cancer pain, acute injuries, and other forms of pain, and it is regarded as the most potent antipyretic, aminophenazone known for its antipyretic and anti-inflammatory properties, has been utilized in breath tests to assess cytochrome P-450 metabolic activity in liver function evaluations.

On the other hand, pyrazole serves as a versatile lead compound for developing potent bioactive agents. It is esteemed for its adaptable framework, making significant contributions to various sectors of the chemical industry, including medical and agricultural fields.[5]

With the rising incidence of cancer, scientific research focused on cancer morbidity, mortality, and improving the quality of life for cancer patients is expanding rapidly. Cancer remains a major health concern across all societies, regardless of wealth or social status.

Continuing our work on the development of new biologically active compounds,[6,7] we present the synthesis of novel pyrazolone derivatives that incorporate both pyrazole and pyrazolone pharmacophores within a single scaffold. This was achieved via the Knoevenagel condensation between 1,3-diaryl-4-formylpyrazoles and 3-methyl-1-phenyl-1H-pyrazol-5-(4H)-ones (**Schema 1**). The anticancer activity and molecular docking studies of these derivatives are also discussed.



Schema 1. Synthesis of pyrazolone derivatives.

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Preliminary DFT calculation and chemical reactivity of natural extracted flavonoids with molecular modelling targeting acetylcholinesterase AChE receptor

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Molecular modeling, powered by advanced computational methods, is revolutionizing the development of new drugs from both natural and synthetic resources. These theoretical approaches enable researchers to identify and refine natural bioactive compounds as promising lead candidates in drug discovery, thereby enhancing the likelihood of success in developing highly effective-targeted treatments.

In our current investigation, we applied density functional theory DFT calculations at the B3LYP/6-311G (d) level to three key flavonoids (**P1**, **P2**, and **P3**) mainly derived from Chinese medicinal plants [1,2]. Structure optimization, frontier molecular orbitals (HOMO and LUMO), and chemical reactivity descriptors were explored, analysed and discussed.

Given the high *in vitro* acetylcholinesterase AChE inhibitory activity of compound **P2** [3] and the promising results obtained from its electronic properties through DFT calculations, molecular docking was performed using AutodockVina, targeting Human AChE (PDB ID:7XN1). Correlating the electronic behaviour and reactivity of **P2** with its biological effect was essential. Consequently, strong hydrophobic and hydrophilic interactions were established between **P2** scaffold and the active amino acids of AChE pocket, forming a complex with a binding affinity of -9.7 kcal/mol. **P2** arranged similarly with the standard drugs donepezil and tacrine.

In conclusion, these theoretical studies provide novel insights into the reactivity of the selected flavonoid **P2** as a potent AChE inhibitor, which aligns with experimental findings.

Keywords: DTF calculations, flavonoids, chemical reactivity, docking, AChE.

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An Investigation into antibacterial and antifungal properties of a medicinal plant belonging to the Fabaceae family

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Chemodiversity found in plants offers valuable resources that could be beneficial for identifying new leads in drug discovery. Fabaceae as the third largest family of flowering plants **(Ahmad, 2016)** was chosen to investigate its antibacterial and antifungal activity. In order to investigate the antimicrobial property of this medicinal plant, two extracts chloroform and ethyl acetate are tested. They were obtained by maceration using solvents with increasing polarity. The antimicrobial activity of the extracts was determined using the agar disk diffusion assay **(Treki, 2009)**.

Evaluation of antibacterial activity revealed that both the CHCl3 and AcOEt extracts showed inhibition zones against Gram (+) bacteria: *Staphylococcus aureus* ATCC 6538 and *Bacillus Spizizenii* ATCC 6633, as well as against the yeast *Candida albicans* ATTC 10231, while they exhibited no inhibition zones against Gram (-) bacterial strains: *Escherichia coli* NCTC 10538 and *Pseudomonas aeruginosa* NCIMB 8626, and even against the fungus *Alternaria alternata*.

Regarding the antibacterial activity, the lowest MIC value of the chloroform extract is observed against *Bacillus Spizizenii* at 6.25 mg/ml, followed by *Staphylococcus aureus* at 50 mg/ml. The MIC values for the ethyl acetate extract are 6.25 mg/ml and 25 mg/ml against *Staphylococcus aureus* and *Bacillus Spizizenii*, respectively.

Concerning antifungal activity, the MIC recorded against *Candida albicans* is lower for the chloroform extract (25 mg/ml) than the ethyl acetate extract (50 mg/ml). These results

suggest that this plant possesses antimicrobial properties that could justify its use in traditional medicine and make it potential source for developing new antimicrobial agents.

Keywords: Fabaceae, Extracts, Antibacterial, Antifungal, MIC.

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An efficient synthesis of a new serie of 1,4-dihydropyridine derivatives

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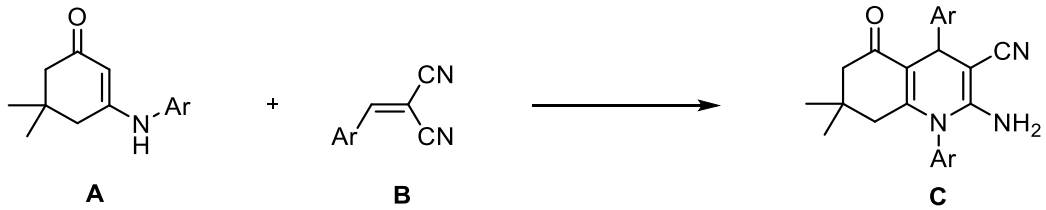
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Abstract

Heterocyclic compounds have one or more hetero atoms in their structure and are of very much interest in our daily life. They may be cyclic or non cyclic in nature. Heterocyclic compunds have a wide range of application and are predominantly used as pharmaceuticals, as agrochemicals and as veterinary products. [1]

1,4-Dihydropyridines (DHPs) are one of the most important classes of heterocyclic compounds as privileged pharmacophores. They are therefore attractive synthetic targets of organic chemistry. Multicomponent reactions (MCRs) are the most efficient strategies for the synthesis of 1,4-DHPs in terms of providing both sufficient structural diversity and numbers for compound libraries. Following the classical multicomponent synthesis of 1,4-DHPs by the Hantzsch reaction, chemists have developed a large number of new MCRs to access 1,4-DHPs with significantly extended structural diversity, which is pivotal for the process of discovering new lead compounds and drugs of 1,4-DHPs. [2-3]

In this work, we report our preliminary results on the synthesis of 1,4-dihydropyridines C by Hantzsch reaction between an unknown enamine A of dimedone and benzylidene malonitrile B under standard conditions.



A **B** **C**

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Synthesıs and characterization of organic molecule with antıbacterıal activity

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The preparation of the Schiff base was finished from condensation reaction between acetophenone and sulfamerazine. The mixture was left under reflux for 2 hours. After cooling in at room temperature; the mixture was cooled in an ice bath for a few minutes. After a few days; crystals shaped needles have been obtained.The FTIR spectrophotometer Perkin Elmer recorded the spectra within the range of 4000 to 400 $cm^{-1}$was used to confirm the structure of the obtained compound. The FTIR spectra typically showed a characteristic peak in 1636 cm^{-1} which is indicative of the C=N group. The antibacterial efficacy of this compound was also tested on two different types of bacteria *Escherichia coli* and *Saccharomyces cerevisiae* using disc diffusion method. The Schiff base derivative showed a good efficiency for all types of tested bacteria strains. The obtained compound could be used as a good antibacterial agent.

Keywords—Schiff base, infrared spectroscopy, biological effect, bacterium, structural study.

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APPLICATION OF DFT TO THE DETERMINATION OF METAL-METAL SPIN-SPIN COUPLING CONSTANTS IN $M2(HNCHNH)_4$ MOLECULES WITH M=Nb, Mo, Tc, Ru, Rh, Pd.

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The correlation between structures and magnetic properties of bimetallic complexes is an extremely active area of research; we are interested in the calculation of Spin-Spin $^1J_{M-M}$ coupling constants in bi-nuclear complexes containing Metal-Metal bonds such as $M2(HNCHNH)_4$ [**1**].

The ADF2006.01 code based on the DFT (Density Functional Theory) **[2]** was used for the calculation of the Spin-Spin coupling constants, in a non-relativistic and relativistic framework.

The first step of our work consists in presiding the optimization of the molecular geometry, using the relativistic framework based on the four functionals BP86, PW91, BLYP, supporting the TZP base and a middle core.

We have calculated the Spin-Spin coupling constants $^1J_{M-M}$ relative to the nuclei Nb, Mo, Tc, Ru, Rh, Pd, taking into account the relativistic [3] effects Zora of scalar and spin-orbit types, while varying the functionals BP, BLYP and revPBE and the three categories of Core.

A comparative study of the results obtained was thus presented.

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Étude phytochimique, activité antioxydante et inhibition des cholinestérases de *Centaurea pubescens* Willd.

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Cette étude porte sur la composition chimique et l'activité biologique de *Centaurea pubescens* Willd., en mettant l'accent sur son potentiel antioxydant et son activité inhibitrice des cholinestérases. L'extrait chloroforme, analysé par chromatographie en phase gazeuse couplée à la spectrométrie de masse (GC/MS), a permis l'identification de 28 composés, parmi lesquels l'arctigénine (33,97 %) constitue le principal constituant. Des quantités notables de l'alcool *trans*-conifèrylique, de loliolide, et d'isovanilline, ces deux derniers composés étant rarement rapportés dans le genre *Centaurea*. L'extrait acétate d'éthyle s'est révélé riche en polyphénols (713,33 mg équivalent acide gallique/g) et en flavonoïdes (450,83 mg équivalent quercétine/g). Cet extrait a démontré une activité antioxydante élevée avec des valeurs IC_{50} de 14,16 µg/mL (DPPH), 8,93 µg/mL (ABTS) et 5,55 µg/mL (GOR), ainsi qu'une capacité réductrice significative. Par ailleurs, l'extrait chloroforme a présenté une activité modérée d'inhibition de la butyrylcholinestérase (BChE), avec une valeur IC_{50} de 81,83 µg/mL. Ces résultats mettent en évidence le potentiel de *Centaurea pubescens* Willd. en tant que source prometteuse d'antioxydants naturels et d'agents thérapeutiques, notamment pour des applications neuroprotectrices.

Mots clés: *Centaurea pubescens* Willd., activité antioxydante, activité anti cholinestérase

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Potentiel antimicrobien d'une nouvelle base de schiff N-[(E)-(4-hydroxyphényl)méthylidène]-4H-1-2-triazol-4- amine : Synthèse, Caractérisation, Évaluation Antibactérienne, et analyse de la surface de Hirshfeld.

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Les bases de Schiff sont des composés de formule générale $R_1R_2C = NR_3$ où l'atome d'azote est lié à un groupe aryle ou alkyle. Cette famille de composés est classée selon la nature des radicaux aliphatiques ou aromatiques.

Plusieurs travaux de notre équipe ont été consacrée à la synthèse, l'étude des structures et des propriétés de cette famille de composés. Nous pouvons citer en exemple les travaux de benarous et al (2015), moussa selimane et al (2015), bouhidel et al (2018), maza et al (2020) [1-4].

Nous présentons dans cette étude la structure déterminée par diffraction des rayons X et les propriétés antimicrobiennes sur quatre souches (deux à Gram positif et deux à Gram négatif) d'une nouvelle base de Schiff obtenue au cours de notre travail, qui est formée sur la base d'un cycle triazole et d'un phénol, reliés par une fonction imine C=N.

L'étude des surfaces d'Hirshfeld nous a permis de mettre en évidence l'importance des liaisons hydrogène dans la construction de l'empilement cristallin de cette structure.

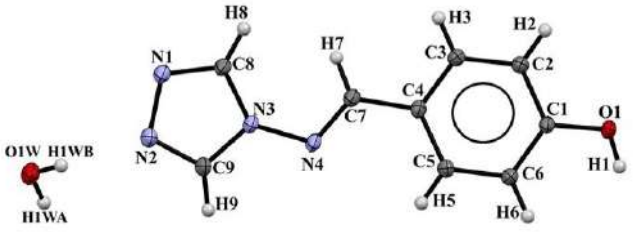


Fig.1: ORTEP of the ligand with thermal displacement ellipsoids drawn at the 50% probability level.

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Indicate the topic of the presentation:

- ✓ **Mathematics**

Numerical ODEs and Numerical PDEs (inc. BVPs)	Probability and Statistics
Applied Algebra and Geometry	Dynamical Systems and Algorithms
Fractional Calculus and its Applications	Complexity Theory, Neural Networks and Fuzzy Systems

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Using Fault Tree analysis in industrial risk analysis for seawater desalination plant

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Safety management based on the risk analysis can enhance the maximum availability and utilization of the technological systems. Fault tree analysis has approved its wide applications in many fields. The present paper takes an example performance evaluation of fault tree analysis method for risk assessment for seawater desalination plant and takes accidental chemical spills as the top event.

A case study of application in seawater desalination plant safety systems illustrates the aim (undesired state to study), principle, the structure of the technique, constructing the fault tree based on AND and OR gates and evaluating the fault tree based on available data, probabilities of occurrences for each event can be assigned, allowing better prevention measures selection and implementation. The Fault Tree Analysis (FTA) is very good tool at showing the logical connections between failure events and the top level hazard or event.

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Crystal structure, FT-IR, ^{1}H and ^{13}C NMR study, and Hirshfeld analysis of 1-[(E)-2-(5-tert-Butyl-2-hydroxyphenyl)-diazen-1-yl]naphthalen-2-ol.

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Azo dyes currently have the highest dye chemistry production volume and in the future their relative significance might further rise, the most significant synthetic colorants, azo dyes are used extensively in the printing, paper and textile, Moreover, in azo dyes the ligands play a crucial role in coordination chemistry and in the construction of functional materials, such as ionophores, self-assembled layers, catalysts, antimicrobial agents, liquid crystals and semiconductors [1]. In this work, we studied an azo compound called: 1-[(E)-2-(5-tert-Butyl-2-hydroxyphenyl)-diazen-1-yl]naphthalen-2-ol was obtained by the reaction of 2-amino-4-tert-butylphenol with β-naphthol and was characterized using single crystal X-ray diffraction studies and spectroscopic methods including FT-IR, NMR ^{1}H and ^{13}C.

The molecule of the title compound, is planar and crystallizes in the monoclinic space group $P2_1/m$. Intramolecular bonds, there are only two types of intermolecular interactions in the crystal structure: strong hydrogen-bonding O–H···N and C–H···O interactions and π–π stacking interactions.

A Hirshfeld surface analysis was undertaken to investigate and quantify the intermolecular interactions. Hirshfeld surface and 2D-fingerprint indicates that the most important contributions to the crystal packing are from H···H (56.7%), C···H/ H···C (20%), O···H/ H···O (10.8%), C···N/ N···C (6.3%) and C···C (4.5%).

Keywords: Azo dyes, spectroscopic methods, X-ray diffraction, Hirshfeld surface, hydrogen bond, π – π interactions.

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Exploring the Phytochemical Composition and Antibacterial Properties of Jacobaea erratica Extracts

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This pharmaceutical chemistry methodological study was conducted to analyze the phytochemical composition and antibacterial properties of the chloroform and methanol extracts from Jacobaea erratica (Bertol.) Fourr., previously known as Senecio erraticus Bertol., a plant species in the family Asteraceae [1].

Qualitative chemical tests were performed to determine the presence of polyphenols, flavonoids, tannins, steroids, and quinones. Steroids, anthraquinones, free quinones, and terpenoids were dominating contents of the chloroform extract, whereas polyphenols, flavonoids, and tannins were dominating in the methanol extract. The extracts were both positive for the presence of glycosides, cardiac glycosides, free quinones, and terpenoids.

The antibacterial activities, which were done by a disc diffusion method with some selected human pathogens (Escherichia coli, staphylococcus aureus, showed that chloroform extract was more effective against Escherichia coli, though methanol extract showed a moderate antibacterial action. The study finds the antibacterial potential was highly significant, and the chloroform extract was effective because steroids, quinones, and terpenoids.

These findings are valuable in the context of pharmaceutical research, emphasizing the potential of J. erratica as a source of natural antibacterial agents.

Keywords: Jacobea erratica; phytochemicals; antibacterial activity; quinones; steroids; terpenoids.

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ANTIOXIDANT ACTIVITY AND FLAVONOIDS OF ETHYL ACETATE EXTRACT OF *Athamanta species*

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The genus *Athamanta* (Umbelliferae) it is kind of flowering plant of the Apiaceae family. consists of about nine species, it is an endemic plant of southeastern Europe and northern Africa (Tomić., 2009), we've been interested with the phytochemical study and antioxidant activity of the ethyl acetate extract of *Athamanta* species.

Air-dried and powdered aerial parts (3000 g) of this species were macerated in a hydromethanol solution (70%) at room temperature. The extract was concentrated to dryness (under low pressure), the residue was dissolved in water and extracted with petroleum ether, chloroform, ethyl acetate and *n*-butanol, successively.

The ethyl acetate fraction (4 g) was subjected to column chromatography on silica gel, eluted with a gradient of *n*-hexane/acetone (0:100) in increasing polarity. Two flavonoids were separated and characterized by the spectroscopic methods 1D experiments (^{1}H,^{13}C) (Mabry et al., 1970; Jay & Gonnet., 1974).

The ethyl acetate extract was tested for its antioxidant activity using four methods (ABTS, Reducing power and Phenanthroline). This extract showed a high activity in ABTS (IC_{50}: 8.97 ± 0.97 µg/mL µg/mL), Reducing power ($A_{0.5}$: 41.72±0.63 µg/mL) and phenanthroline ($A_{0.5}$: 9.60 ± 0.18 µg/mL) assays.

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Photocatalytic Degradation of Chromium by Ruddlesden-Popper La_2NiO_4: A Pathway for Industrial Wastewater Treatment

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Abstract

This study investigates the photocatalytic properties of the perovskite La_2NiO_4 for the degradation of aqueous pollutants. The material was synthesized via the citrate route and characterized using various techniques. Results showed that La_2NiO_4 possesses a direct bandgap of 1.42 eV, rendering it active under solar irradiation. When coupled with tin oxide (SnO_2), this material demonstrated the ability to reduce chromate ions to chromium III ions. The use of salicylic acid as a hole scavenger significantly enhanced the efficiency of the photocatalytic reaction [1].

Keywords: La_2NiO_4, photocatalysis, chromate, reduction, tin oxide, salicylic acid.

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Relativistic DFT study of the magnetic properties of diuranuim U(IV)-U(IV) ethynediyl-bispyrazine and imino-amido quinoid complexes

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Molecular materials with magnetic and/or optical properties have garnered significant interest in both experimental and theoretical research. At the molecular level, f-element organo-polymetallic complexes, such as actinides linked by functionalized ligands bridging paramagnetic centers, exhibit magnetic exchanges of either ferromagnetic or antiferromagnetic nature. The concept of magnetic super-exchange, introduced by O. Kahn [1a], laid the groundwork for the development and synthesis of numerous magnetic molecular materials, ultimately leading to the discovery of Single Molecular Magnets (SMM) [1b].

The theoretical investigation of magnetic behavior in such systems is challenging, but advancements in computational power and quantum methods, particularly Density Functional Theory (DFT) and the broken symmetry (DFT-BS) approach developed by Noodleman et al. [2], have enabled several studies to illuminate the ferro- and antiferromagnetic properties of diuranium diimide magnetic compounds, such as the diimide complexes [Cp_3UV] (μ-L) (L = stilbene-, naphthalene-diimide) [3]. This magnetic behavior is influenced by the bridging ligand and the structural environment of the metal centers.

Our works focuses on the theoretical study of the magnetic properties of f-element molecular complexes bridged by functionalized ligands, specifically diuranium complexes with ethynediyl-bispyrazine and imino-amido quinoid ligands. Using the relativistic DFT/ZORA/TZP method with the B3LYP hybrid functional and the AMS (Amsterdam Modeling Suite) code, we found that the DFT/ZORA/B3LYP/BS approach accurately reproduces the magnetic behavior of these compounds. Our study highlights the critical role of 5f orbitals in metal-ligand interactions and U($5f^2$)-L-U($5f^2$) electronic communication, which is crucial for magnetic exchange. The BS approach confirmed the antiferromagnetic interaction between U(IV)-U(IV) centers, in agreement with experimental observations.

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Antioxidant and antimicrobial activities of some new synthesised 1H-Benzimidazoles

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Over the years of active research in organic and medicinal chemistry, fused nitrogen heterocycles have long been recognized as essential targets because of a possibility of synergy of biological properties or the induction of other properties not present in each of the heterocycles tested separately.

Among these heterocycles, we are interested in benzimidzolylimidazopyridine compounds.

Indeed, Benzimidazoles constitute an interesting pharmacophore in drug design and discovery due to their multiple biological activities (antimicrobial, antiparasitic, antihistaminic, anticancer, antiallergic and antioxidant). [1]

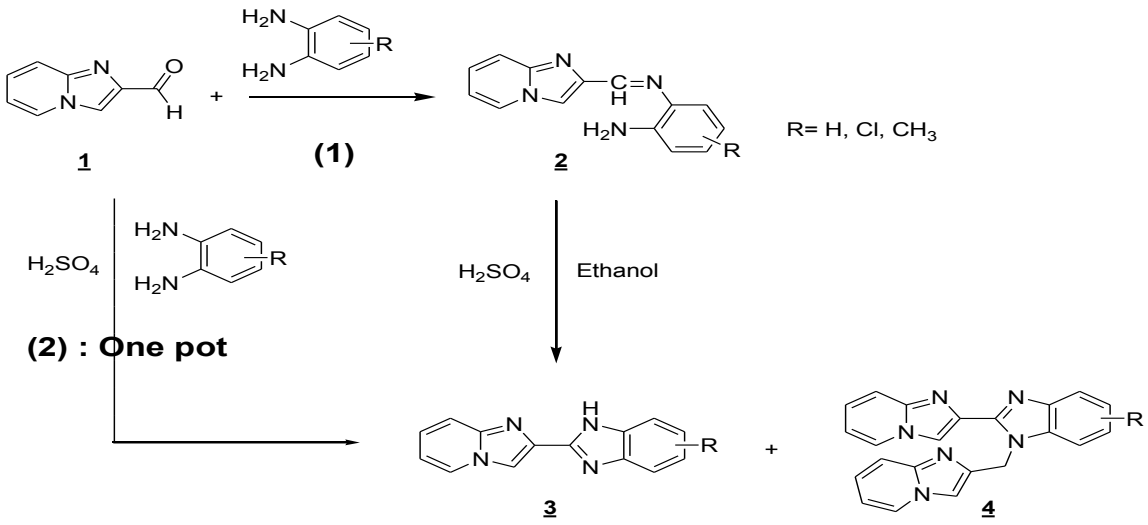
On the other hand, imidazo [1, 2-a] pyridine is a nitrogen bicycle known for its pharmacological effects. [2]

In this present study we report the synthesis of a serie benzimidazole compounds 3 as described in scheme 1.

The one-pot synthesis of these same compounds yielded a secondary product: the N-substituted bezimidazoles 4.

The antioxidant activity of the synthesized compounds was evaluated by the DPPH radical reduction method using ascorbic acid as a reference. Antimicrobial activity was performed in vitro against Staphylococcus aureus, Eschericha coli and Candida albicans strains using the gel diffusion method.

Keywords: Heterocycle, imidazo[1,2-a]pyridine, benzimidazole , antioxidant, antimicrobial.



Scheme 1: Synthesis of benzimidazoles.

References:

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Photodégradation d'un phytorégulateur à la surface des plantes

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La dégradation induite par le rayonnement solaire est une voie importante de la dissipation des pesticides dans l'environnement. Il se peut même que ce soit le processus majeur pour certains pesticides dans les eaux de surface. Cependant, la photodégradation est rarement prise en compte à la surface de la végétation après pulvérisation des cultures [1].

Dans ce travail nous nous somme interessé au sel de calcium de l'acide 3-oxido-5-oxo-4-propionylcyclohex-3-enecarboxylique qui contribue à réguler la croissance végétale [2]. L'étude a été réalisée en solution et en solide.

Après sa pulvérisation, le composé étudié passe un temps plus ou moins long à la surface des feuilles de plantes et peut se phototransformer. Il se photolyse aussi bien en solution qu'en phase solide. En milieu aqueux et en présence de H_2O_2, la substance active est instable. Son élimination totale du milieu peut intervenir dans l'heure qui suit son épandage. La dégradation par les triplets de la phénalénone est particulièrement efficace. Par contre, en milieu solide, la phénalénone et le H_2O_2 ont un effet inhibiteur. Dans les deux milieux étudiés le même photoproduit a été détecté par HPLC.

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Theoretical study of the structure and optical properties of transition metal complexes based on Bis{1-[(o-tolyl)iminomethyl]-2-naphtholato}.

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Our research focuses on the study of complexes based on nickel and copper. The calculations were performed using time-independent density functional theory (DFT) and time-dependent DFT (TD-DFT). The aim is to calculate the structural and energetic properties, as well as the UV-Visible absorption spectra, using two functional: CAM-B3LYP [1] and LC-M06L [2], along with the QZVP basis set.

The calculations are performed using the GAUSSIAN 09 program and the graphical interface developed by A. R. Allouche, called GABEDIT [3].

The obtained results better reproduce the experimental data, and the comparison between the experimental absorption spectrum and the calculated absorption spectra indicates that the functional that best matches the experimental results is the hybrid functional B3LYP. However, the corrections of the two functional, CAM-B3LYP and LC-M06L, have no influence on our results. Therefore, the functional used are the parameters that influence the calculation of the energy gap, regardless of the basis set employed.

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PHYTOCHIMICAL ANALISIS OF ALGERIAN PLANT *Astragalus gombo*

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Abstract
The genus *Astragalus* contains about 3000 species and represents one of the largest genus in the family of Fabaceae (Heywood, 1978) This genus is represented in Algeria by about 40 species, including *Astragalus gombo* Coss. & Dur. This endemic perennial plant grows in sandy arid and desert pastures of Algeria
Two flavonoides were isolated from the butanol soluble part of the hydroalcoholic extract of the aerial parts of Astragalus Desf. (fabaceae), an endemic species of the North of Sahara. The structures of this compound has been elucidated on the basis of extensive 2D NMRspectroscopic analyses, including COSY, TOCSY, NOESY, HSQC, CIGAR-HMBC, H2BC and HSQC-TOCSY.

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HPLC analysis and antioxidant activity of a plant hydrosol belonging to the Rubiaceae family

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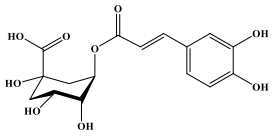
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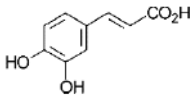
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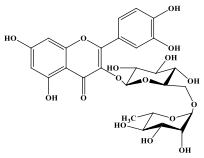
The Rubiaceae family, known for its pharmacological properties, is rich in secondary metabolites such as anthraquinones, iridoids, triterpenes, alkaloids, and flavonoids [1]. This chemical diversity makes them a promising source of new bioactive agents.

The objective of this study is to identify, for the first time, the chemical compounds present in the hydrosol extracted from the dried aerial parts of a plant from *Asperula* genus of the Rubiaceae family, using HPLC analysis. Additionally, the antioxidant activity of this extract will be evaluated to explore the plant's potential to neutralize free radicals.

HPLC analysis of the plant's hydrosol revealed a significant presence of chlorogenic acid (1), caffeic acid (2) and rutin (3) as structures demonstrated in figures.


(1)


(2)


(3)

The antioxidant activity of hydrosol extract was assessed using two techniques: the ferric reducing antioxidant power test (FRAP), which gave a value of **233.5 mg TE/100 g** dried plant, and the free radical neutralising capacity test (ABTS), with a value of **202.163 mg TE/100 g** dried plant.

The results of this study revealed a significant antioxidant effect, particularly in neutralizing free radicals and reducing iron, due to the presence of phenolic compounds. These findings pave the way for future research into its pharmacological and therapeutic applications.

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Synthesis of high-value aroma chemicals *via* enzymatic bioacylation

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Flavors and fragrances esters, constitute important ingredients in food, beverages, cosmetics, pharmaceuticals, fine chemicals, perfumes, body lotions, face creams, shampoos, soaps, shower-shaving gels, and other toiletries, due to their olfactory properties [1]. Among them, aromatic flavors and fragrances acetates are endowed with great fruity and floral smell and taste, which contributes to their tremendous applications in the food, pharmaceuticals, and cosmetic industries. Among them we quote: phenyl, benzyl and phenethyl acetates are of outstanding interest [2]. These acetates can be obtained from natural sources, since they are present in plants, such as jasmine and gardenia; however, its direct extraction and purification are highly complex and expensive [3].

In order to resolve this problem and according to the increase demand for greener, environment-friendly processes, biocatalysis seems the ideal solutions affording this valuable acetate. Furthermore, enzymatic methods are labeled as natural in accordance with the United States and European Legislations, thereby satisfying the consumer trend towards natural products in various industries [4].

In this context, herein, we describe the impact of the modulation of some parameters on the efficiency of the enzymatic acylation of benzyl alcohol as model of study such: the amount and lipase nature lipase nature, the acyl donor and the reaction time. The optimal conditions are applied for the bioacylation of phenol and 2-phenylethanol.

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Méthode efficace pour la préparation de benzamides contenant une fraction sulfonamide en utilisant l'hétéropolyanion de Preyssler

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La fraction benzamide joue un rôle crucial dans la structure de nombreux composés bioactifs, offrant une variété considérable de caractéristiques biologiques et curatives [1-3].

De plus, les dérivés sulfonamide ont démontré une efficacité pharmacologique significative dans le traitement de diverses affections [4, 5]. Grâce à leur prix modéré, leur toxicité réduite et leur potentiel thérapeutique remarquable, ces médicaments sont fréquemment utilisés pour prévenir et soigner diverses infections chez les individus.

La convergence de deux composants bioactifs donne naissance à une nouvelle molécule prometteuse en tant que composé principal dans les efforts de découverte de médicaments.

Dans cette optique, une application catalytique simple et rapide de l'hétéropolyacide de Preyssler pour la synthèse des benzamides contenant une fraction sulfonamide a été rapportée dans ce travail.

Cette méthode se déroule en une seule étape, comprenant la déprotection et la benzoylation des *N*-(tert-butoxycarbonyl) sulfonamides pour donner les composés cibles avec de bons rendements (jusqu'à 92 %).

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Herbicide-induced enzymatic activity inhibition in tyrosinase/CoC_3N_4/SPCE biosensor for the detection of acetamiprid

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Herbicides are widely used in agriculture to protect crops from diseases, insects, and weeds. However, only a fraction of the herbicides used reach their target, while the rest can seep into the soil, leading to the contamination of ground and surface water resources [1,2].

Given the growing interest in on-site detection of analytes that can replace traditional techniques, electrochemical sensors offer a low-cost and convenient solution for detecting various analytes. These sensors are widely used in agriculture, food, and petroleum industries, as well as in environmental and biomedical applications [3].

In addition, sensors based on tyrosinase as a biological element have proven to be simple and practical tools for the determination of phenol due to their high sensitivity, efficiency, and simplicity [4].

In this work, we report the stepwise design of tyrosinase/CoC_3N_4/SPCE biosensor for the sensitive detection of acetamiprid. The stepwise surface modification was assessed by cyclic voltammetry, electrochemical impedance spectroscopy and square wave voltammetry.

The modified electrode can selectively detect catechol ranging from 2 to 400 µM with a limit of detection of 0.12 µM. In presence of acetamiprid, the enzyme activity is proportionally inhibited in respect to the herbicide concentration. The biosensor shows linear relationship ($r > 0.996$) of the inhibition levels from 4,5 to 360 nM with a limit of detection of 1,3 nM.

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Boron Removal from Water by Mg-Fe Layered Double Hydroxide: Impact of Calcination.

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In this study, Mg-Fe layered double hydroxide (Mg-Fe LDH) was synthesized via the co-precipitation method with and without calcination at 500°C, and applied for boron removal from aqueous solutions. XRD analysis confirmes the lamellar structure of the LDH prepared without calcination. The results of batch experiments demonstrate that in the two cases, boron removal efficiency increases with the pH increase to reach a maximum at pH: 9,5. Whatever the preparation mode of the LDH, the removal kinetics is well described by the second-order and Elovich models, and the equilibrium data follow both the Langmuir and Freundlich models. The calculated parameters of the used models, suggest that the use of calcination in the preparation of Mg-Fe LDH, implies a decrease in the removal speed and an increase in the removal capacity.

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Physicochemical characterization and antibacterial activity evaluation of Pyrazolidine/β-cyclodextrin inclusion complex

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Abstract:

Pyrazolidines compounds show various biological and pharmacological activities such as antimicrobial, anti-inflammatory, antitumor, insecticides, analgesic and anticancer activities [1-3]. However, it is poorly soluble in water, and its bioavailability is limited. The aim of this research is to investigate in the host-guest inclusion complexes of Pyrazolidine: β-cyclodextrin using the β-cyclodextrin derivatives to improve their chemical and antimicrobial properties.

The host-guest of binary inclusion complexe of pyrazolidine with polysaccharides β-cyclodextrin and their derivatives was prepared by co-precipitation and freeze drying technicals. The stoichiometric ratio of complexes is 1:1 was calculed by continous variation (Job's plot) and the stable constants of binary complexe calculed by Benesi- Hildebrand method. The host-guest inclusion complexes in the solid state was characterized by infrared spectroscopy (FTIR) and nuclear magnetic resonance spectroscopy NMR (^{1}H, ^{13}C, 2D ROSY) witch revealed the inclusion of this pyrazolidine drug within cyclodextrin cavity. In addition, the morphology and topography of these complexes were performed respectively by MEB and AFM microscopy. The antimicrobial activity of the complexes was measured by against bacterial: Escherichia coli, Staphylococcus aureas, Pseudomonas aeroginosa, Salmonela, Bacillus subtilus spizizenii and fungical: Candida albicans and Aspergilus braziliensis with ATCC references [4].

These investigations improve that the preliminary evaluation of the antibacterial activity using agar disk diffusion methods shows that some of these host–guest inclusion complexes of *Pyrazolidine:β-cyclodextrin* exhibit interesting antimicrobial activity.

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Synthesis, Structural Characterization, and Acetylcholinesterase (AChE) Inhibitors for Alzheimer's Treatment of new Asymmetric Schiff Base

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Typically, a primary amine reacts with a carbonylated substance (aldehyde or ketone) to form a Schiff base. During the synthesis, a water molecule is removed and the carbonyl or aldehyde C=O link to be replaced by C=N [1].
Due to their diverse structures and properties, Schiff bases are used in fields as diverse as organic chemistry, catalysis, biology [2], complexing agents and corrosion inhibitors.

This research work focuses on the synthesis of the new asymmetric Schiff base. This compound was characterized by spectroscopic analysis techniques: Fourier Transform Infrared (FTIR) and Ultraviolet Visible (UV-Vis), and Liquid Chromatography-Mass Spectrometry (LC-MS).

The effective concentration (EC 50) showed that the compound Schiff base has good acetylcholinesterase activity.

Keywords: Synthesis, Schiff base, Effective concentration.

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Characterization of the use of ash for the removal of a triphenylmethan dye

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In the objective to valorize waste products, the present study aims to characterize the removal of the green malachite dye by ash prepared by calcination of sewage sludge. Structural and textural analyses were performed for the characterization of the prepared ash. The dye removal experiments were realized in batch. DRX analysis shows that the obtained fly ash is principally constituted by quartz, calcite and dolomite. The surface area determined by BET analysis is 11,50m2/g. The pHpzc determined by drift method is about 9,35. The results of macroscopic analysis show that the dye removal is maximal at pH<7. The equilibrium time is about 4h. The adsorption kinetics is well described by the second order and Elovich models. The increase in temperature in the range 20°C-40°C, has no effect on the removal kinetic. The removal capacity of the prepared ash determined at pH: 2 by Langmuir equation is about 55mg/g.

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Synthesis of New Salicylaldehyde Derivatives with Enhanced Antioxidant Activity and Potential Cholinesterase Inhibition Capacity

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Salicylaldehyde derivatives are well-known for their broad range of biological activities, including antioxidant and enzyme inhibition properties [1, 2]. Enhancing the antioxidant activity of these compounds is particularly important due to their potential role in neutralizing reactive oxygen species (ROS) and preventing oxidative stress-related diseases [3]. Additionally, inhibiting cholinesterase enzymes, such as acetylcholinesterase and butyrylcholinesterase, is a promising strategy for treating neurodegenerative diseases like Alzheimer's [4]. This study focuses on the synthesis of novel salicylaldehyde derivatives with improved antioxidant properties and the potential to inhibit cholinesterase enzymes, aiming to develop multifunctional bioactive molecules for therapeutic applications.

A series of salicylaldehyde derivatives featuring a secondary amine scaffold were synthesized and fully characterized through spectroscopic techniques. The compounds demonstrated excellent antiradical activity, confirmed by the DPPH assay, and showed strong reactivity towards free radicals, as supported by DFT calculations. Furthermore, molecular docking studies revealed favorable binding affinities for both AChE and BuChE enzymes, highlighting their potential as promising cholinesterase inhibitors.

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Experimental data of salt effect on liquid-liquid equilibrium of the ternary system: water/ phormic acid/ buatanol

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Separation processes such as distillation, extraction, absorption, crystallization, adsorption and membrane processes are of great importance in various industrial sectors (chemicals, pharmaceuticals, petrochemicals, refining, etc.). The diversity of the types of separation that can be achieved has widened considerably [1]. Among these separation processes, the most widely used is solvent extraction. This can be defined as a separation technique which takes advantage of the difference in solubility of the constituents of a homogeneous liquid charge in a suitable solvent [2]. Knowledge of liquid-liquid equilibria is essential for the design and evaluation of extraction processes and gives an economic indication of the use of solvents, whose task is to modify partition coefficients to achieve high separation factors.

The addition of a salt to an aqueous solution can significantly change the equilibrium composition of a given system. The representation of these liquid-liquid equilibria (in the presence of either electrolytes or salts) is particularly complex, due to the nature of the physicochemical phenomena involved, as well as the partial or complete dissociation of the salts. This is known as the “salt effect”.

This effect can therefore be exploited to influence immiscibility curves by increasing or decreasing the area delimited by the binodal curve, and to influence the inclination of the slopes of the bond lines linking phases in equilibrium.

In this context, the present study focuses on the effect of salts on the liquid-liquid extraction of formic acid from an aqueous solution using butanol as the solvent. The presence of the salt introduces ionic forces which directly influence the widening of the immiscibility curve and the distribution of the solute between the extract and raffinate phases, leading to "salting-out" and "salting-in". Liquid-liquid equilibrium data for ternary systems (Water/Formic acid/Butan-1- ol) in the presence and absence of two salts NaCl and CaCl2 at different percentages (5%, 10%, 15%) were determined experimentally at room temperature and atmospheric pressure using the cloud point method. The experimental results demonstrated the influence of the different salts on the liquid-liquid equilibria of the ternary system studied, and that the presence of salt modifies this equilibrium in favor of the extracted phase. The reliability of the experimental data obtained was successfully verified by the application of Othmer-Tobias [3] and Hand correlations.

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Synthesis of hybrid organic/inorganic composite based on natural adsorbent: an economical and sustainable approach for water remediation

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Adsorption is a process that is attracting a great deal of interest from researchers around the world because of its efficiency and eco-environmental benefits. but the use of chemically or thermally modified adsorbents involves high energy consumption or the use of expensive chemicals that are harmful to the environment. That is why the use of adsorbents in their natural state is a very promising alternative. but the separation of these natural adsorbent from the treated solutions is also a costly operation in terms of energy. hence the need for an innovative solution which is the incorporation of magnetic materials such as magnetite for the synthesis of biomaterial/magnetite composites.

In our work, we have compared a natural material and its magnetic composite in the adsorption of organic pollution presented by cationic dye and heavy metals also the comparison of process cost were examined in order to assess the cost of magnetization compared with the benefits of this operation. The results obtained showed that the efficiency of the biomaterial increased after magnetization, due to the adsorption capacity of the incorporated magnetite and through an economic analysis of the process we find that more than 50% of energy consumption has been saved with the use of the composite material as adsorbent.

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Optimization of operating parameters for the synthesis of a green nanomaterial

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Abstract :

The main sources of water pollution are industrial effluents containing toxic and hazardous substances. These include dyes from the textile industry. These substances cause unprecedented damage to the environment.

To solve these problems, various treatment methods have been employed. The most promising are adsorption processes.

Nanomaterials play a crucial role because, at this scale, they present emerging characteristics that could have a major impact in many fields. Green nanomaterials are materials synthesized by green synthesis using plants.

In this work, we synthesized an MgO nanomaterial by green synthesis using Pistacia lentiscus leaf extract.

The study focused on optimizing the operating parameters for the magnesium oxide (MgO) nanomaterial, including variations in: the concentration of the extract and the concentration of the precursors used. Optimization was carried out using adsorption tests with an organic dye (methylene blue).

Key words: Adsorption; water pollution; nanomaterial; green synthesis.

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One-pot, multi-component synthesis of ethyl 2-(4-formylphenyl)-4-methyl-1H-benzo[b][1,4]diazepine-3-carboxylate derivatives and its application

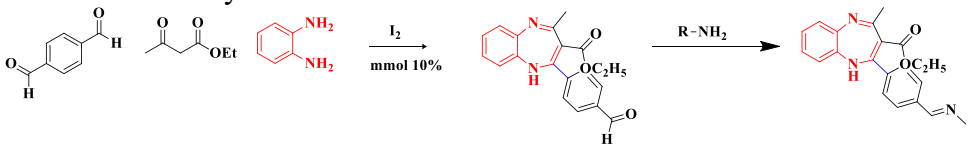
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Abstarct

Compounds with seven-membered heterocycles containing nitrogen atoms are of interest due to their significant biological and pharmacological properties. Benzodiazepines and their derivatives have shown therapeutic and pharmacological potential for various diseases, leading to increased focus on their synthesis in medicinal chemistry. The chemistry of benzo-hetero-azepines and their derivatives has recently become a new research area. Seven-membered compounds and their derivatives are significant in the heterocycle family as they are present in important biological molecules. One-pot reactions using terephthalaldehyde aldehydes with o-phenylenediamine and ethyl acetoacetate yield an intermediate that can be further reacted with various amines, including o-phenylenediamine and aminophenol. This approach allows for the formation of complex polyheterocyclic compounds by integrating additional nitrogen and oxygen functionalities, offering diverse pathways for the synthesis of bioactive heterocycles.



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Infrared Spectroscopy Analysis of Polymeric Materials Synthesized Chemically

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In this work, we present the essential factors for synthesizing two different types of polymers through chemical synthesis methods (emulsion polymerization and polycondensation). We also discuss their chemical and physical properties, including solid phase, solvent, time, concentration, and temperature.

The first polymer was synthesized from distilled styrene in the presence of $K_2S_2O_8$ at a temperature of 70-90°C, yielding polystyrene with a good efficiency of 61.28%. The second polymer is a phenolic copolymer obtained via polycondensation in an acidic medium at 80°C, using sulfuric acid as a catalyst, for 3 hours. Sulfonation of these macromolecules with sulfuric acid (97%) is a necessary step to create a strongly acidic cationic function. Due to the exothermic nature of the reaction, it is maintained at room temperature under stirring in a cooling bath until the total addition of the acid.

Chloromethylated polystyrene was obtained through two successive and complementary steps: chloromethylation of the polymer at 58°C, followed by amination at 60°C [1-5].

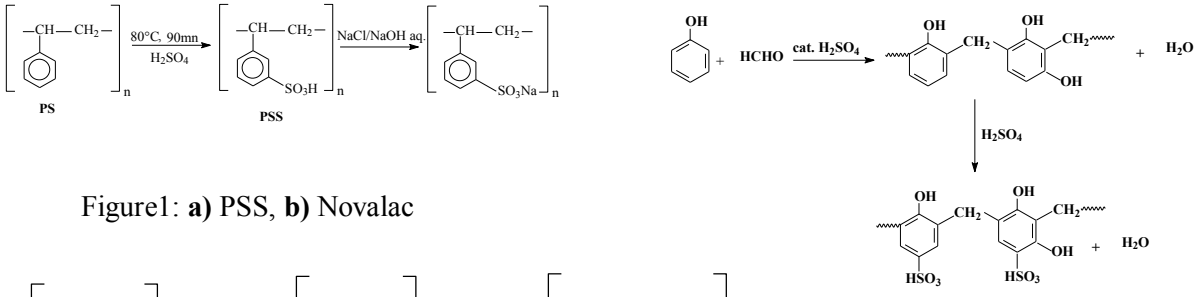


Figure1: **a)** PSS, **b)** Novalac

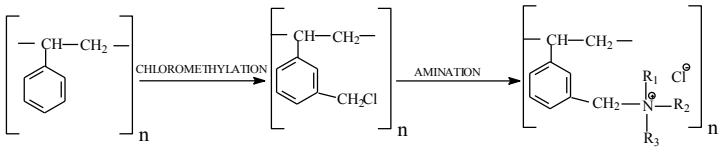


Figure2: PS Chloromethylated

These polymeric materials are used in the preparation of ion-exchange materials (either anionic or cationic), with a wide range of applications, particularly in water treatment.

Styrene: ν_{C-H} = 3031.9-3058.9-3024.2 cm^{-1} (aromatic ring) / $\nu_{C=C}$ = 1627.8 cm^{-1} (vinyl group)
$\nu_{C=C}$ = 1573.8-1496.7 cm^{-1} (aromatic ring)/$\nu_{C=C}$ = 987.5-910.3 cm^{-1} (vinyl group)
ν_{C-H} = 786.9 cm^{-1} (aromatic ring)/ $\nu_{C=C}$ = 684.3 cm^{-1} (aromatic ring)

Polystyrene: ν_{C-H} = 3082.0-3058.9-3024.2 cm^{-1} (aromatic ring) /ν_{C-H} = 2920 cm^{-1} (asymmetric) - 2850.6 cm^{-1} (symmetric) (methylene group) $\nu_{C=C}$ = 1450.4-1492.8 cm^{-1} (aromatic ring)

Chloromethylated Polystyrene: ν_{C-H} = 3082.0-3058.9-3028.0 cm^{-1} / ν_{C-H} = 2923.9 (asymmetric) - 2850.6 cm^{-1} (symmetric) (methylene group) / $\nu_{C=C}$ = 1600.8-1450.4-1492.8 cm^{-1} (aromatic ring)
ν_{C-H} = 1153.4 cm^{-1} (-CH_2Cl group) / ν_{C-H} = 1180.4-1315.4 cm^{-1} (methylene group)
ν_{C-H} = 1068.5-1026.1 cm^{-1} (aromatic ring) / ν_{C-Cl} = 797.0 cm^{-1} (-CH_2Cl group)

Chloromethylated Polystyrene (after amination) ν_{C-H} = 3082.0-3058.9-3024.2 cm^{-1} /$\nu_{C=C}$ = 1600.8-1492.8-1450.4 cm^{-1} (aromatic ring) ν_{C-N} = 1261.4 cm^{-1} / ν_{C-H} = 1369.4 cm^{-1} (methyl group)

Synthesized Novolac: ν_{C-H} = 1091.6 cm^{-1} (methylene group) / $\nu_{C=C}$ = 1473.5-1508.2 cm^{-1} (aromatic ring)/ ν_{C-OH} = 3421.5 cm^{-1} (phenolic group)

Sulfonated Novolac: ν_{C-H} = 1091.6 cm^{-1} (methylene group) / $\nu_{C=C}$ = 1473.5-1508.2 cm^{-1} (aromatic ring)/ ν_{C-OH} = 3421.5 cm^{-1} (phenolic group)/ ν_{C-S} = 617.2 cm^{-1} / $\nu_{S=O}$ = 1180.4-1373.2 cm^{-1}

These polymeric materials are used in the preparation of ion-exchange materials (either anionic or cationic), with a wide range of applications, particularly in water treatment.

Keywords: Styrene, polymerization, FTIR, copolymer, polymer, polycondensation.

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Photocatalytic reduction of hexavalent chromium (Cr(VI)) using $ZnFe_2O_4$ Spinels

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This research work focuses on evaluating the photocatalytic properties of zinc ferrite ($ZnFe_2O_4$) spinel for the degradation of aqueous pollutants, particularly chromate ions (CrO_4^{2-}). The $ZnFe_2O_4$ was synthesized via the nitrate method and characterized using various techniques (XRD, FTIR, DR). Results showed that $ZnFe_2O_4$ exhibits a direct bandgap of 1.57 eV, conferring photocatalytic activity under solar irradiation. When coupled with zinc oxide (ZnO), this material effectively reduced chromate ions to chromium III ions (Cr^{3+}) in a photoelectrochemical system. The addition of salicylic acid as a hole scavenger significantly enhanced the efficiency of the photocatalytic reaction by limiting the recombination of electron-hole pair[1].

Keywords: $ZnFe_2O_4$, photocatalysis, chromate, reduction, zinc oxide, salicylic acid.

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Synthesis and theoretical study of novel cyclic imides containing sulfonamide moiety as carbonic anhydrase type II inhibitors using green methods: Molecular docking and ADME prediction

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Cyclic imides and sulfonamides represent a significant class of compounds with notable potential for inhibiting carbonic anhydrase isoenzymes (CAs)[1,2], which play crucial roles in various physiological and pathological processes. These compounds inhibit CA activity by interacting with the enzyme's active site, where the sulfonamide moiety binds to the catalytic zinc ion, effectively blocking enzymatic function. Additionally, cyclic imide containing structures, such as succinimide, maleimide, and phthalimide, exhibit diverse biological activities[3] and their combination with a sulfonamide moiety may result in potent carbonic anhydrase inhibitors.

Our research focuses on synthesizing novel cyclic imides derivatives that incorporate sulfonamide group, employing a solid catalyst and ultrasound irradiation[4].

To examine interactions between the synthesized molecules and human carbonic anhydrase II (PDB IDs: 2AW1, 3SH4), as well as their pharmacokinetic properties, we conducted molecular docking studies and ADME predictions.

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Chemical composition and anticancer activity of the essential oil extracted from fresh and dried aerial parts of *Vicia ochroleuca* Ten.

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Abstract: The search for new bioactive substances with anticancer activity and the understanding of their mechanisms of action are high priorities in the research effort toward more effective cancer treatments. In this article, we analyzed, for the first time, the chemical composition of the essential oil (EO) hydrodistilled from the aerial parts of *Vicia ochroleuca* Ten. (Leguminosae) by GC–MS. A total of sixteen compounds representing 82.2% of the total composition were identified. The major compounds were phytone (20.11%), hexadecanoic acid (10.23%), 1-octen-3-ol (9.84%), and 10-epi-α-cadinol (7.13%). Additionally, using the MTT (3-[4,5-dimethylthia-zol-2-yl]-2,5-diphenyltetrazolium bromide) method, the EO was tested *in vitro* against a panel of human cancer cells, including breast (MDA-MB 231), colon (HCT116), melanoma (A375), and glioblastoma (T98G), with corresponding IC_{50} values of 23.07, 47.05, 51.64, and 64.07 lg/mL, respectively. The results demonstrate cytotoxic activity and suggest that *V. ochroleuca* EO could be regarded as a natural bioactive source.

Keywords: *Vicia ochroleuca*, essential oil, anticancer activity.

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Phytochemical investigation of *Anacyclus pyrethrum*

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The *Anacyclus* genus, belonging to the Asteraceae family and native to the Mediterranean region, includes around thirteen species, recognized since ancient times for their medicinal properties and as a source of bioactive compounds, including flavonoids, terpenoids, coumarins, and steroids (Aliboudhar *et al*., 2015; Side Larbi *et al*., 2017).

To explore new bioactive substances, a phytochemical investigation was undertaken on the species *Anacyclus pyrethrum*, leading to the isolation and structural identification of four compounds.

The isolation process involved several chromatographic methods, including silica gel and Sephadex LH-20 column chromatography, and preparative TLC chromatography.

The structures of the isolated compounds were determined through various spectroscopic techniques, such as 1D NMR (^{1}H, ^{13}C), 2D NMR (COSY, HSQC, HMBC), mass spectrometry, and also by comparison with existing literature.

Keywords: *Anacyclus pyrethrum*; Asteraceae; coumarins; spectroscopic techniques.

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Synthesis, X-ray diffraction and Hirshfeld surface analysis of new hybrid compound: $[SnF_6]^{2-}$, $2(C_8H_{12}NO)_2^+$, H_2O

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In recent years, the attention in organic–inorganic compounds have increased. In general, the combination of two extremely different components provides a way to design new hybrid materials as well as additional properties can be introduced, which the individual inorganic or organic components do not have, such as electronic, optical magnetic and ferroelectric properties etc... This valuable features of hybrids, open promising new pathways for the use in a very broad application areas like catalysis, non-linear optical response (NLO), development of new pharmaceutical drugs etc… [1].

Tyramine is a monoamine compound derived from the amino acid tyrosine. Tyramine occurs widely in plants and animals and is metabolized by the enzyme monoamine oxidase. In fact, it is often produced by the decarboxylation of tyrosine during fermentation or decay. This is somewhat similar in its action to adrenaline in raising blood pressure and stimulating smooth muscles [2].

A new hybrid compound ($[SnF_6]^{2-}$, $2(C_8H_{12}NO)^+$, H_2O), has been obtained by the reaction of tin fluoride with tyramine in acidified water, and was isolated from a slow evaporation reaction at ambient temperature. Crystal structure was determined by single-crystal X-ray diffraction analysis. It crystallizes in the monoclinic system with P $2_1/c$ space group and the following lattice parameters: a = 7.5294(5)Å, b= 23.3824(15) Å, c = 11.5388(7) Å with Z = 4. The three-dimensional ionic structure of this compound consists of alternating layers of inorganic anions and organic cations. They are linked together by cation–anion, cation-water, water -cation, water -anion hydrogen bonds and the dominant non-covalent interactions have been quantified using Hirshfeld surface analysis.

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STRUCTURAL CHARACTERIZATION AND HIRSHFELD ANALYSIS OF $[Pb(Imid)_4NO_3]NO_3$ COMPLEX

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Keywords: Imidazole, X-ray Diffraction, coordination chemistry and hirshfeld analysis.

Abstract

The crystal structure of $[Pb(Imid)_4NO_3]NO_3$ (Imid = imidazole $C_3H_4N_2$) has been determined by X-ray diffraction on monocristal. The title compound $[Pb(C_{12}H_{16}N_8)NO_3]NO_3$ contains four imidazole molecules and two nitrate ions. The lead(II) ion is coordinated by four N atoms from four imidazole rings and one O atom from nitrate ion. The structure of the molecule may be described as $Pb(Imid)_4NO_3$ square pyramidal deformed. The three imidazole rings and one NO_3 forme a base equatorial plane. The Pb-N bridge distance and terminal Pb-O bonds are in the range of 2.424 Å - 2.609 Å and 2.889 Å respectively and are in good agreement with those found in organometallic compounds $[Pb(C_{10}H_6N_3O_4)(H_2O)_2].2H_2O$ (Guo et al. 2014) and $[Pb(C_5H_2N_2O_4)(H_2O)]$ (Zhang et al. 2006). The crystal packing is stabilized by weak N-H…O and N-H…N interactions.

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Theoretical Study of Cyclophosphamide Inclusion by β-Cyclodextrin

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Abstract

Cyclophosphamide is a widely used anticancer agent, but its low solubility and significant side effects limit its therapeutic efficacy. To address these issues, this study explores the inclusion of cyclophosphamide within supramolecular hosts such as β-cyclodextrin. This approach aims to enhance the drug's solubility and stability while reducing its adverse effects.

The objective of this study is to theoretically model the inclusion of cyclophosphamide by β-cyclodextrin, analyzing the energetic and structural properties of the resulting complexes to determine their stability and potential applications in pharmacology.

The modeling was conducted using Gaussian software, employing the B3LYP (6-31G(d,p)) method to optimize the geometries of the inclusion complexes. The structures of the hosts and cyclophosphamide were constructed and optimized, followed by an in-depth analysis of the non-covalent interactions involved in the inclusion process.

The simulations indicate that the inclusion of cyclophosphamide by β-cyclodextrin is thermodynamically favorable, with complexation energies suggesting the formation of stable complexes. Molecular orbital analyses and hydrogen bonding interactions further confirm the high stability of these complexes, making this approach promising for enhancing cyclophosphamide's therapeutic efficacy.

The inclusion of cyclophosphamide within β-cyclodextrin shows significant potential to improve drug delivery by increasing its solubility and reducing side effects. This theoretical study provides a solid foundation for future experimental research aimed at developing new pharmaceutical formulations based on supramolecular complexation.

Keywords: cyclophosphamide, β-CD, DFT, Non-covalent interactions.

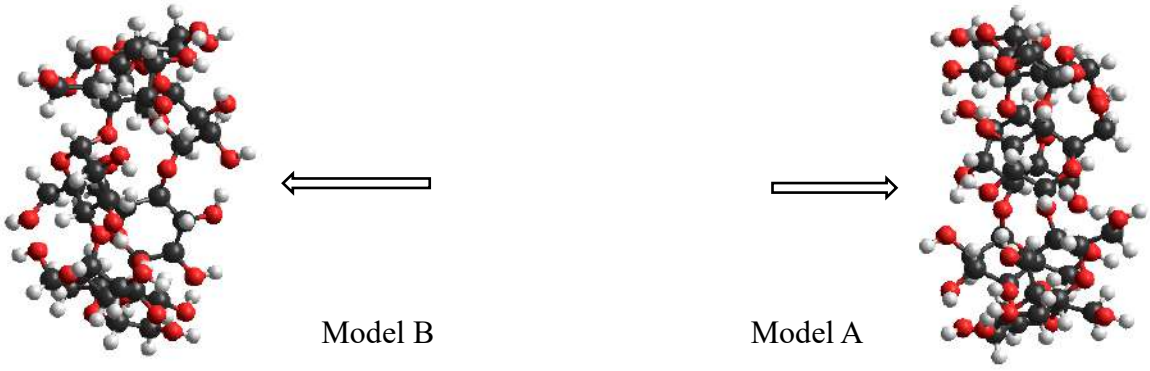


Figure: Coordinate system used to define the inclusion process of cyclophosphamide in β-CD.

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Chemical and electrochemical synthesis and characterization of rGO- NiO-PANI ternary composites.

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Reduced graphene oxide (rGO), a derivative of graphene, has attracted significant interest due to its exceptional properties such as high specific surface area, excellent electrical conductivity, and mechanical strength. However, its limited functionalization can restrict its practical applications. To overcome these limitations, we propose the integration of rGO with polyaniline (PANI) a conductive polymer and nickel, a transition metal. The incorporation of PANI is expected to enhance the composite's electronic properties, while the addition of nickel can improve its conductivity and chemical stability, opening up new possibilities for energy storage, catalysis, and sensing applications.

Initially, we synthesized reduced graphene oxide (rGO) from graphite using two methods: electrochemically, using KOH as an electrolyte, applying a voltage of 10 V, and chemically, using the modified Hummers method in two steps: oxidation of graphite to graphene oxide (with $KMnO_4/H_2SO_4$) and reduction of graphene oxide to rGO using hydrazine as a chemical reducer.

Additionally, we produced rGO-NiO-PANI composites incorporating nickel and polyaniline through chemical and electrochemical techniques, including cyclic voltammetry. Conductivity and solubility tests, Fourier Transform Infrared Spectroscopy (FTIR), UV-Visible spectroscopy, and cyclic voltammetry were used to characterize the synthesized products.

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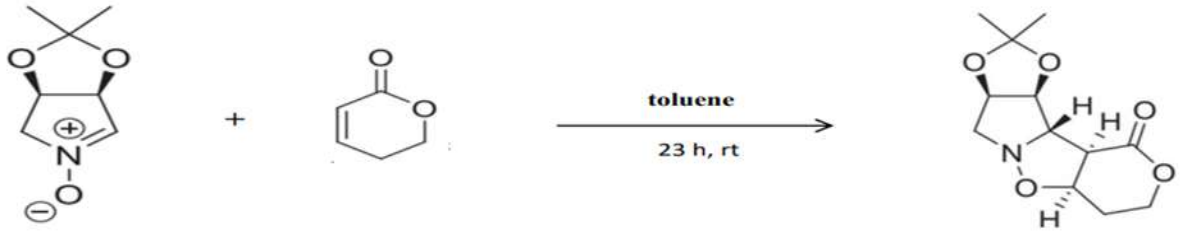
Regio- and stereoselectivity of the [3+2] cycloaddition of nitrones with α,β-unsaturated lactones : A DFT investigation.

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The B3LYP/6-31+G(d,p) DFT method was used for the study of the mechanism and the regioselectivity and stereoselectivity of the [3+2] cycloaddition reaction between α,β-unsaturated lactones with nitrone. In gas phase and toluene, this [3+2] cycloaddition reaction is characterized by a completely meta region-and stereoselectivity.The analysis of the thermodynamic characters indicates that by the inclusion of the experimental conditions, the reaction becomes endergonic and thereby under thermodynamic control favoring the formation of the most stable product as observed experimentally. The analysis of the global electron density transfer (GEDT) at the transition states and bond order (BO) show that this reaction takes place via one-step synchronous and non-polar mechanism. While local Parr functions analysis allows us to explain the meta region-and stereoselectivity observed experimentally.



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Synthesis and Biological Evaluation of new Dihydrospiro[indoline-3,4'-pyrazolo[3,4-d]pyrimidine]

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A novel series of dihydrospiro[indoline-3,4'-pyrazolo[3,4-d]pyrimidine]-based compounds has been synthesized through a multi-step synthesis route. The synthesized compounds were evaluated for their biological activities, including [specific biological activity, e.g. antioxidant, anti-inflammatory, antimicrobial, .The results showed that several compounds exhibited potent activities. The molecular structure and biological activity of the compounds were analyzed using various techniques, NMR spectroscopy,and mass spectroscopy. The findings of this study suggest that these dihydrospiro[indoline-3,4'-pyrazolo[3,4-d]pyrimidine]-based compounds have promising potential drugs.

Keywords: dihydrospiro[indoline-3,4'-pyrazolo[3,4-d]pyrimidine], synthesis, biological evaluation, antioxidant, anti-inflammatory, antimicrobial

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Contribution aux contrôles physicochimique des huiles essentielles commercialisée dans la wilaya de Tizi Ouzou

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L'aromathérapie est une forme de médecine alternative qui utilise les huiles essentielles (HE), substances volatiles et extrêmement concentrées présentes dans les plantes, pour améliorer le bien- être physique, mental et émotionnel. L'utilisation des HE ne se limite pas à l'aromathérapie ; elles sont également employées dans divers secteurs tels que la cosmétologie, l'agroalimentaire et les produits d'hygiène. Malgré leurs propriétés thérapeutiques, les HE sont hautement toxiques et peuvent provoquer des effets indésirables néfastes. Elles sont contre-indiquées dans certaines situations, notamment chez les enfants, les femmes enceintes et dans certains cas de maladies comme l'asthme et l'épilepsie.

Une réglementation stricte et un contrôle rigoureux sont donc indispensables. L'absence d'une réglementation stricte en Algérie pour ces substances à intérêt thérapeutique croissant complique leur contrôle, rendant difficile la garantie de leur qualité et de leur sécurité.

Dans ce contexte, nous avons effectué un contrôle de neuf échantillons d'huiles essentielles disponibles sur le marché de la wilaya de Tizi Ouzou : huiles de citronnelle de Java, de clou de girofle, d'eucalyptus globuleux, de lavande, de menthe poivrée, de romarin, de sauge sclarée, de thym et de zest d'orange. Ce contrôle a été réalisé selon les normes de la 11ème édition de la Pharmacopée Européenne, ainsi que les normes ISO et AFNOR spécifiques à ces produits. Notre contrôle a porté sur l'emballage, l'étiquetage, ainsi que sur les caractéristiques organoleptiques (odeur, couleur, aspect) et physico- chimiques (indice de réfraction, pouvoir rotatoire, densité, indice d'acide, indice de peroxyde, indice de saponification, et indice d'ester, etc.).

Nos résultats ont révélé une absence d'informations essentielles sur l'emballage et l'étiquetage de tous nos échantillons, tels que le nom botanique, les précautions d'utilisation, les contre-indications spécifiques et le numéro de lot. Cette lacune peut induire les consommateurs en erreur. De plus, la non-conformité aux conditions de remplissage, comme le sous-remplissage des flacons, peut accélérer l'altération des HE. En ce qui concerne les caractéristiques organoleptiques et les essais physico-chimiques, ils étaient conformes à la 11ème édition de la Pharmacopée Européenne ainsi qu'aux normes ISO (chapitre ISO/TC54) pour les huiles suivantes : citronnelle de Java, eucalyptus globuleux, lavande, menthe poivrée, romarin, sauge sclarée et thym. Cependant, nous avons observé un indice de peroxyde élevé pour les échantillons de clou de girofle et de zest d'orange, probablement dus au sous-remplissage ou à de mauvaises conditions de stockage.

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Corrosion inhibition of salts derivatives for API 5L Gr.B steel in corrosive media

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In industrial applications, metals are exposed to acidic solutions. Hydrochloric acid and sulfuric acid are the most common types of aggressive solutions for these applications. This is a costly materials science problem dating back to the days of metal discovery [1]. Therefore, it is essential to add corrosion inhibitors to the metals subjected to these liquids in order to prevent metal corrosion [1]. For a long time, organic compounds have been recognized as corrosion inhibitors for metals in acidic media [2]. The majority of well-known inhibitors are organic molecules containing N, S, or O atoms organic compounds with functional electronegative groups and p electrons in triple or conjugated double bonds are also employed, allowing them to adsorb to the metal surface and create protective complex layers [3].

The objective of this research to evaluate the corrosion inhibition efficiency of some Imidazolium salts. The corrosion rate and the efficiency of the studied compound on the corrosion of API 5L Gr.B steel sample in 0.5M H_2SO_4 with different concentrations and at various temperatures was measured by weight loss method. The tested compounds were effective as corrosion inhibitors for steel in sulfuric acid, and IE was dependent on the length of chain attached to nitrogen atoms.

Keywords: Imidazolium salts, API 5L Gr.B steel, Weight loss, Corrosion.

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Synthesis, Investigation of Inhibitory Effects , and Theoretical Modelling of Azines: An Integrated Approach Using Molecular Docking, Density Functional Theory, and X-Ray Diffraction

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Azines, specifically N-N linked diimines (R-CH=N-N=CH-R), represent an important functional class of Schiff bases that has gained increasing attention in recent years. The azine motif has proven its significance and effectiveness as a privileged substructure found in a wide range of biologically active molecules, including those with anticholinesterase and antioxidant activities.

This study aims to investigate the inhibitory activity of substituted azines on acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). Initially, we will carry out the synthesis and characterization of azines, employing X-ray diffraction (XRD) to determine their crystalline structures. The inhibitory effects will then be assessed through inhibition tests, allowing us to measure IC_{50} values for each ligand.

Simultaneously, a theoretical approach integrating molecular docking and density functional theory (DFT) will be adopted. Molecular docking will facilitate the study of ligand-enzyme interactions, while DFT calculations will provide insights into the electronic properties of the ligands and the associated inhibition mechanisms.

The results of this research will help identify the most effective ligands and deepen our understanding of the structure-activity relationships of azines. This work could also open avenues for the development of new inhibitory molecules with potential therapeutic applications in the treatment of neurodegenerative diseases.

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Extraction of *Marrubium vulgare L.* and in vitro evaluation of their antioxidant and anti-inflammatory activities

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Our study focused on the cold maceration extraction of the Mediterranean plant *Marrubium vulgare*, aiming to isolate its bioactive molecules for medicinal use. Known commonly as horehound, *M. vulgare* is a perennial herb of the *Lamiaceae* family that has been used traditionally to treat respiratory and gastrointestinal ailments. The plant is rich in marrubiin, a labdane diterpene, as well as phenolic acids, flavonoids, and other bioactive compounds that contribute to its medicinal properties [1].

For our research, we fractionated the crude extract into several fractions, including cyclohexane, chloroform, ethyl acetate, butanol, and water fractions. Subsequently, we quantified the polyphenols and flavonoids in these fractions and evaluated their antioxidant and anti-inflammatory activities.

M. vulgare has demonstrated significant antioxidant potential, supported by various assays such as DPPH and FRAP, which revealed that phenolic-rich fractions effectively scavenge free radicals, a property beneficial for countering oxidative stress and reducing the risk of chronic diseases like diabetes and cardiovascular conditions [2].

In the DPPH assay, the crude extract exhibited strong antioxidant activity, with an IC_{50} below 8 µg/mL. Notably, the butanol fraction displayed an IC_{50} below 1 µg/mL in the ABTS assay, along with $A_{0.5}$ values below 40 µg/mL in the FRAP assay and below 30 µg/mL in the Phenantroline assay. The aqueous extract also showed higher anti-inflammatory activity, with an IC_{50} of approximately 102.61 µg/mL, surpassing the standard diclofenac (IC_{50} = 128.43 µg/mL), aligning with research suggesting M. vulgare's efficacy in reducing pro-inflammatory markers [3].

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Nicotinamide, a promising insulin secretagogue agent

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Diabetes is a serious global health issue brought on by insufficient insulin secretion or improper insulin utilization by the body which results in chronic hyperglycemia. The disease is associated with multiple severe complications primarily affecting the kidneys, heart, and eyes. Numerous medications have been developed to manage this illness and thereby mitigate its complications. Even through their effectiveness, these medications have a number of negative effects that restrict their use, necessitating the search for novel natural molecules. Given its various biological properties, nicotinamide, which is a food-derived vitamin, has attracted great interest. Taking this into account, we carried out this investigation to assess nicotinamide's potential as an antidiabetic by examining its effect on insulin secretion using mice isolated islets. For this, the Langerhans islets of BALB/C mice were isolated following the collagenase digestion procedure. Nicotinamide at a concentration of 60 ug/ml was evaluated for its effect on mouse-isolated islet viability and on glucose-stimulated insulin secretion from these later using the trypan blue colorimetric assay and the Sandwich insulin ELISA kit, respectively. Our in vitro experiments have demonstrated that nicotinamide (60ug/ml) significantly potentiates glucose-stimulated insulin secretion in mice-isolated islets (***$p<0.001$) compared to islets cultured in the RPMI-1640 alone. Parallely, nicotinamide at the same concentration did not affect islet cell viability. This rules out the possibility that the rise in insulin secretion in nicotinamide-treated islets is caused by cell lysis.To conclude, nicotinamide may be a promising candidate for an alternative antidiabetic therapy, and it deserve further investigations.

Keywords: Nicotinamide, Insulin secretagogue, Islet viability, Antidiabetic therapy .

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Eucalyptus-Mediated Green Synthesis of Silver-Doped ZnO Nanoparticles for Enhanced Photocatalytic Degradation of Methylene Blue

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The increasing demand for sustainable solutions to environmental pollution, particularly for water treatment, has driven research into green nanomaterials for photocatalysis. Heterogeneous photocatalysis, owing to its ability to effectively degrade organic pollutants, is recognized as a leading advanced oxidation process. Zinc oxide (ZnO), a widely studied semiconductor, has garnered significant attention in this field because of its favorable electronic properties, low cost, and wide availability. Doping ZnO with metals like silver (Ag) can further enhance its photocatalytic efficiency[1].

This study presents a novel, eco-friendly synthesis of silver-doped ZnO (ZnO-Ag) nanoparticles using eucalyptus leaf extract as a natural reducing and stabilizing agent. This green synthesis method utilizes phytochemicals in Eucalyptus extracts to control nanoparticle formation[2]. Our comprehensive characterization revealed that the optimized 5% Ag-doped ZnO nanoparticles exhibited a narrow size distribution and enhanced light absorption properties. These nanoparticles demonstrate significantly higher photocatalytic activity for methylene blue (MB) dye degradation under UV irradiation than undoped ZnO. Remarkably, Ag-doped ZnO degraded 97.6% of MB within 60 min, a substantial improvement over the 79.2% degradation achieved by undoped ZnO. The mechanism of the enhanced photocatalytic activity was elucidated through detailed kinetic studies and radical-scavenging experiments.

This green synthesis method for Ag-doped ZnO nanoparticles demonstrates a promising approach for developing cost-effective and environmentally friendly water treatment solutions with potential applications in large-scale water purification systems.

Keywords: Green synthesis; Silver-doped ZnO nanoparticles; Eucalyptus leaf extract; Photocatalysis; Methylene blue degradation; Water treatment; Eco-friendly nanomaterials

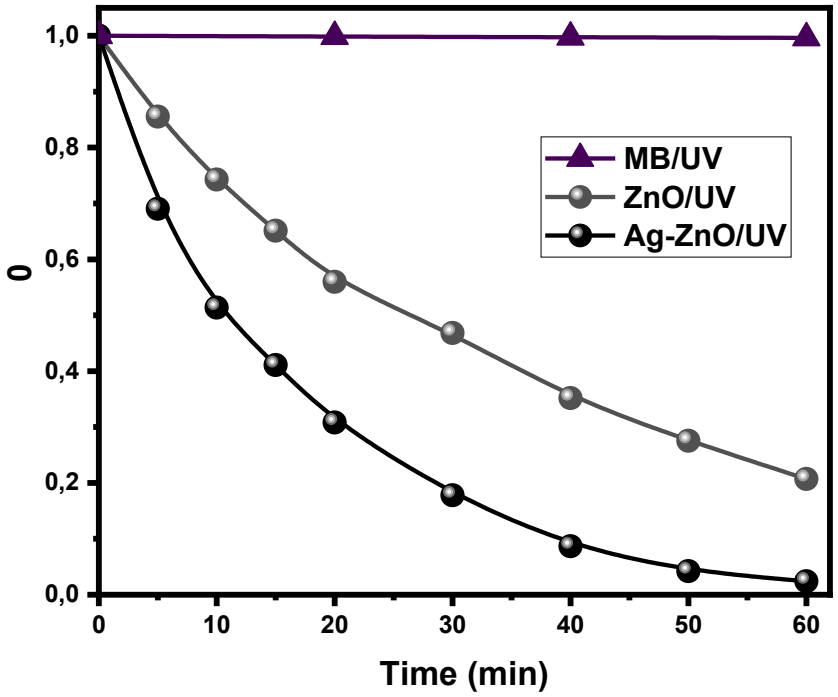


Figure 1: MB photocatalytic degradation with UV-irradiation in the presence of undoped and Ag-doped (5%) ZnO

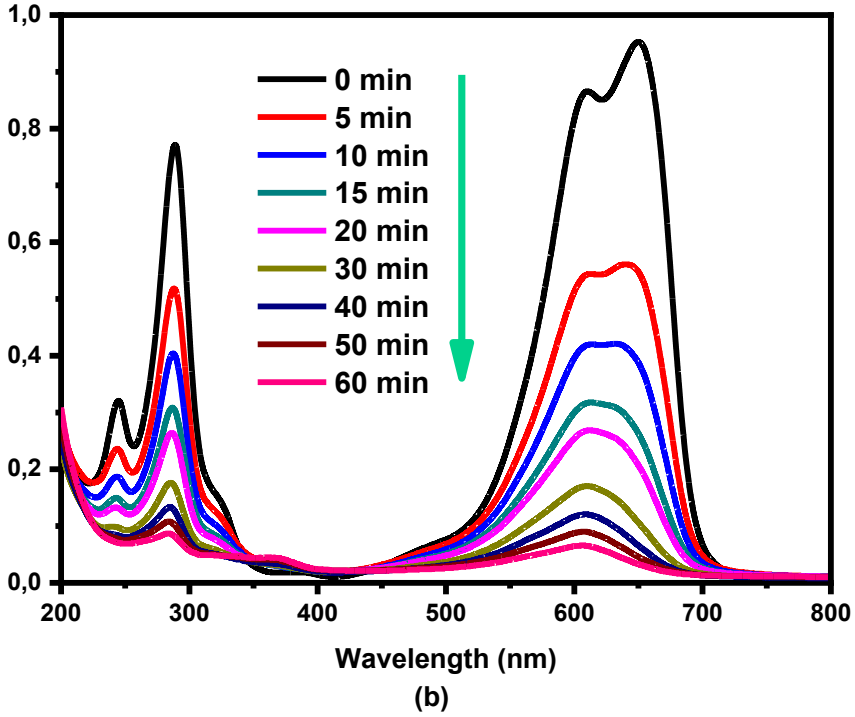


Figure 2: MB absorption spectra after different UV-irradiation time using Ag-doped (5%) ZnO.

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Exploration of Anticholinesterase and Antioxidant Activities in Phenolic-Pyridinic Derivatives: Synthesis, In Vitro Evaluation, and In Silico Studies

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Abstract

Acetylcholinesterase (AChE) is a key enzyme in the nervous system responsible for hydrolyzing acetylcholine, thus terminating its signaling activity. This regulatory mechanism is essential for cholinergic transmission, which is involved in various cognitive and neuromuscular processes. AChE inhibition is a widely used therapeutic approach for the treatment of diseases such as Alzheimer's and myasthenia, as it aims to enhance cholinergic activity to improve cognitive functions or muscle strength. AChE inhibitors bind to the enzyme's active site, preventing the breakdown of acetylcholine and thus prolonging its effect [1]. In the search for new derivatives exhibiting acetylcholinesterase (AChE) inhibitory potential, a series of 24 phenolic-pyridinic derivatives were synthesized and evaluated for their antioxidant activity. A molecular modeling study was conducted to assess their inhibitory capacity against AChE. In silico analyses further demonstrated a promising affinity of these compounds for the active sites of the targeted enzymes. These findings indicate that the synthesized compounds exhibit notable antioxidant properties and significant therapeutic potential.

Keywords : Antioxidant activity, Acetylcholinesterase, Phenolic-pyridinic derivatives, Molecular modeling.

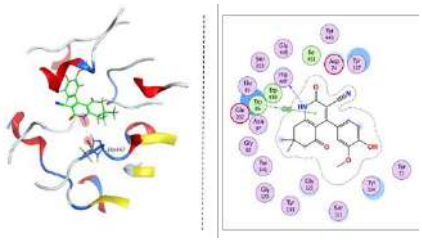


Figure. Interaction modes of the best candidate with AChE.

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Synthèse et évaluation de l'activité antibactérienne et anti-inflammatoire d'une nouvelle série de N'-benzylidene-7-(benzyloxy)-6-methoxy-2-methylquinoline-3-carbohydrazide

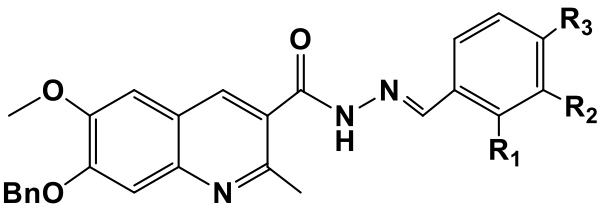
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La quinoléine est un hétérocycle azoté bien connu et présent dans de nombreux produits naturels bioactifs et médicaments. Il s'agit d'un fragment pharmacophore important doté d'un large éventail d'activités biologiques. En effet, de nombreux médicaments sur le marché incluent ce noyau[1]. D'autre part, les bases de Schiff, notamment le benzylidène benzohydrazide, sont des entités chimiques au potentiel thérapeutique avéré [2].

L'objectif du présent travail est de créer une entité chimique hybride combinant les deux entités (quinoléine et benzylidène benzohydrazide) pouvant mener à de nouvelles propriétés biologiques très utiles [3]. D'où ressort l'idée de synthétiser une nouvelle série de N'-benzylidène quinoléine benzohydrazides (Figure 1) via une synthèse multi-étape à partir de la vanilline comme précursseur. Lors du processus de synthèse nous avons essayé d'adopter des protocoles verts et d'utiliser des catalyseurs peu polluants. Le but ultime fut l'évaluation de l'activité antibactérienne et anti-inflammatoire des molécules cible (Figure 1).



6a-h: R_1=H, R_2=H, R_3=H, OH, OMe, Me, NMe_2, NO_2, Cl, Br
6i : R_1=H, R_2=OMe, R_3=OH
6j : R_1=OH, R_2=H, R_3=H

Figure 1: Structure générale des nouveaux N'-benzylidene-7-(benzyloxy)-6-methoxy-2-methylquinoline-3-carbohydrazides.

Le test évaluant l'activité antibactérienne des composés synthétisés a été réalisé contre 5 souches de bactéries de référence (ATCC) dont une bactérie Gram-positive, Staphylococcus aureus, et trois bactéries Gram-négatives : Escherichia coli ATCC25922, Klebsiellapneumoniae ATCC700721 et Klebsiellaoxytoca ATCC8724, ainsi que Bacillus subilis ATCC 6633. Trois médicaments antibactériens ont été utilisés comme référence, la ciprofloxacine (quinolone), l'amikacine et la gentamicine (deux aminosides). L'évaluation a été réalisée à l'aide de la méthode de diffusion sur gélose, également connue sous le nom de méthode de diffusion sur disque. Trois paramètres ont été déterminés, les diamètres d'inhibition, la CMI (concentration minimale inhibitrice) et la CMB (concentration minimale bactéricide) [4].

Les composés synthétisés se sont avérés être actifs vis-à-vis de deux souches bactériennes (Escherichia coli ATCC25922 et Bacillus subilis ATCC 6633) quelques composés étaient bactéricides et d'autres étaient bactériostatiques.

D'autre part, l'évaluation de l'activité anti-inflammatoire *in vivo* des composés synthétisés a été menée sur des souris femelles albinos sur lesquelles on provoque un œdème sur la patte arrière avec injection de solution 1% de carraghénane, selon une méthode (adaptée) décrite par Winter et al. en 1962 [5]. Le diclofénac, un médicament AINS, a été utilisé comme référence. Les résultats montrent que la plupart des composés cibles ont montré une activité anti-inflammatoire très marquée en inhibant efficacement l'œdème provoqués par le carraghénane.

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Inhibition the corrosion of aluminum in 0.5 M HCl medium by the use of a coordination polymer

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Corrosion is a harmful phenomenon, which consists of the destructive attack of a metal by chemical or electrochemical reaction with its environment. It reduces its properties, making it unusable for an expected application. Corrosion inhibitors are generally used to prevent corrosion. They can help stop or slow down the corrosion of a metallic material.

In this work, we were interested in evaluating the effectiveness of a coordination polymer ([Sr(C5H6O4)(NO3)(C3H5N2)(H2O)]n) as a corrosion inhibitor for aluminum in 0.5M HCl medium, using pontentiodynamic polarization. The compound studied was synthesized using a specific method, and characterized by single-crystal X-ray diffraction.

The results of this study showed that the effectiveness of this compound depends on its concentration and the temperature of the corrosive medium. The best inhibition rate reached 84.17% in the presence of 5×10-3 M of the inhibitor at 55°C. Electrochemical tests showed that the studied compound acts as a cathodic inhibitor at 25, 35 and 45°C, and behaves as a mixed inhibitor at 55°C. The inhibitor adsorbs on the aluminum surface according to the Langmuir model by forming mixed bonds (physical and chemical) with a chemical predominance.

Keywords: Coordination polymer, corrosion inhibition, aluminum alloy, hydrochloric acid, polarization curves.

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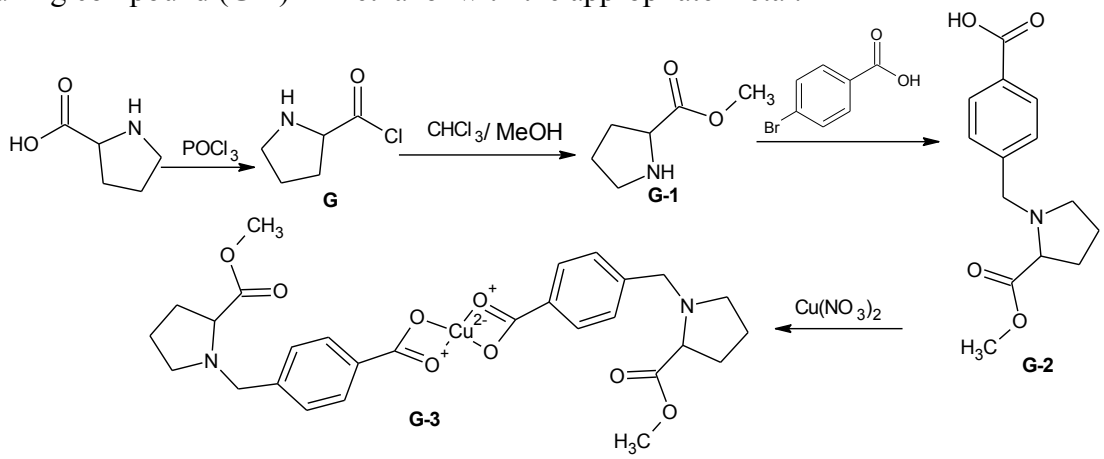
Synthesis and Structural Analysis of Schiff Base Complexes for Antibacterial Applications

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Recent studies have highlighted the chemistry of amino acids and azole derivatives, emphasizing their biological significance and potential applications in pharmaceuticals and biology [1,2]. Their metal complexes are of particular interest, prompting the development of synthesis methods for these compounds [1]. Metal complexes offer a versatile platform for designing novel therapeutic agents and play essential roles in the pharmaceutical industry and agriculture [3]. The target compounds (G-3) were synthesized through a multi-step process, beginning with the esterification of pyrrolidine-2-carbonyl chloride with methanol. The resulting ester was then reacted with 4-bromobenzoic acid in a mixture of 60% acetone and 40% water to produce compound (G-2). Finally, the products (G-3) were obtained by refluxing compound (G-2) in methanol with the appropriate metal.



The obtained products were characterized by various spectroscopic methods, including **IR , UV and NMR (H1, C13).**

The chemical substances were synthesized in our laboratory; they were then tested for the purpose of enhancing its antibacterial capacities **against gram negative bacteria (Klebsiella pneumoniae ATCC700603, Citrobacter freundii ATCC8090, Salmonella typhi ATCC13311, Enterobacter cloacae ATCC13047) and gram positive bacteria (Staphylococcus aureus ATCC25923.**

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Comparative Study of Gentian Violet Dye Removal by Adsorption Using Eggshell-Derived Bioadsorbent and Commercial Nanoparticles

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Abstract

In this study, we present an experimental investigation on the removal of Gentian Violet dye from a solution through adsorption using two different materials: a bioadsorbent derived from egg shell waste and a commercially available nanoparticle adsorbent.

The egg shell waste was used in its natural state after washing, drying, and grinding, within a batch reactor. Several factors influencing the retention capacity were studied, including the effect of contact time, pH, and the solid-liquid ratio.

Adsorption isotherms were used to describe the dye adsorption process, and the B.E.T model showed the best correlation coefficient. Kinetic models, such as the pseudo-first order and pseudo-second order, were applied to analyze the data obtained for dye adsorption.

The results indicated that the bioadsorbent followed the pseudo-first order model, while the commercial nanoparticle adsorbent followed the pseudo-second order model.

Keywords : Gentian Violet dye, Traitement water, Bioadsorbent, Nanoparticles, Adsorption isotherms

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Optimization of cobalt and nickel removal using liquid–liquid extraction by D2EHPA

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ABSTRACT

Solvent extraction stands as a fundamental process in the nickel extraction industry, providing a sophisticated means of separating and purifying nickel from its ores. As industries strive for greater efficiency and sustainability, the importance of refining nickel extraction techniques has never been more apparent[1-3].

phosphoric acid (D2EHPA, HL) at 25°C has been studied. The research examined the effects of several parameters, including equilibrium pH, extractant concentration, and the type of diluent. The impact of using both polar and non-polar solvents on the extraction of cobalt(II) and nickel is analyzed. It was determined that the extracted cobalt(II) and nickel species are CoL2, NiL2 when using methyl isobutyl ketone, and CoL2.2HL, NiL2.2HL when using chloroform and 1-Octanol. Extraction constants for the various diluents were also evaluated.

Key Words: Liquid-liquid extraction, Cobalt(II), Nickel(II), Di(2-ethylhexyl) phosphoric acid, Diluent effect

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Optimization of Secondary Metabolite Extraction for Pharmaceutical and Parapharmaceutical Chemistry Applications

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Secondary metabolites are bioactive compounds with considerable potential in both pharmaceutical and parapharmaceutical chemistry, valued for their therapeutic effects, such as antimicrobial, antioxidant, and anti-inflammatory properties. However, the efficient extraction of these metabolites presents challenges due to their structural diversity, plant origin, and the influence of environmental growth factors. This study aims to optimize extraction parameters—specifically solvent type, temperature, and extraction duration—to maximize the yield and purity of targeted metabolites. The optimization process identified effective conditions for achieving high-quality extracts, suitable for pharmaceutical and parapharmaceutical use. This scalable protocol supports the availability of valuable secondary metabolites, facilitating further research and application in product development for health-related industries.

Keywords : Secondary Metabolites, Extraction Optimization, Pharmaceutical Chemistry

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Etude structurale et analyse de surface Hirshfeld d'un nouveau complexe de cuivre à base du ligand 2-(2-aminophenyl)-1H-benzimidazole.

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Au cours de ces dernières décennies, la chimie hétérocyclique est devenue le centre d'intérêt d'une large communauté de chimistes et théoriciens. Deux tiers des composés organiques, connus dans la littérature qui sont des hétérocycles à trois et à quatre chaînons [1] et contenant de l'azote, inhibent différentes enzymes, sont le pharmacophore de médicaments, ou sont considérés comme des médicaments candidats dans de nombreuses thérapies [2]. Les composés hétérocycliques à noyaux benzimidazole [3] qui est qualifié comme « clé principale » en raison de son excellent profil biologique et de ses applications multiples en chimie médicinale, est l'un des composés hétérocycliques à activité multiples connus dans la littérature. Il fait partie des cinq hétérocycles azotés aromatiques à cinq membres les plus courants dans les médicaments pharmaceutiques approuvés par la FDA américaine (Food and Drug Administration) [4].

La chimie des composés métalliques du bloc d est importante dans différents domaines telles que la chimie analytique, la chimie inorganique, la catalyse ou l'extraction des métaux [5]. La coordination des ions métalliques aux entités organiques ou minérales donne naissance à des complexes de coordination.

Notre objectif est d'étudier la coordination à un métal de transition d'un ligand dérivé du benzimidazole : 2-(2-aminophenyl)benzimidazole, ce qui nous a permis d'obtenir un nouveau complexe de coordination : $[[Cu(2\text{-ampb})_2(H_2O)]^{2+}, SO_4^{2-}]$, que nous allons l'étudier structuralement par diffraction des rayons x et l'effectuer un analyse de surface Hirshfeld.

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Synthesis and Characterization of a Novel Blue Fluorescent EDOT Derivative

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A novel monomer, 4,4'-[(2,3-dihydrothieno[3,4-b][1,4]diorin-5-yl)vinyl]-1,1'-biphenyl (BPE), was synthesized and electrochemically polymerized into poly(4,4'-[(2,3-dihydrothieno[3,4-b][1,4]diorin-5-yl)vinyl]-1,1'-biphenyl) (PBPE). The resulting polymer film was characterized using various techniques, including cyclic voltammetry, X-ray photoelectron spectroscopy, SEM, infrared spectroscopy, and UV-Vis spectroscopy. PBPE exhibits interesting electrochromic properties. When polarized at 0.9 V, the oxidized polymer film appears green and has an absorption band around 670 nm in the UV-Vis spectrum (Figure 29). This absorption band disappears when the film is polarized at -1 V, and a new band appears at 350 nm, resulting in a brown colour.

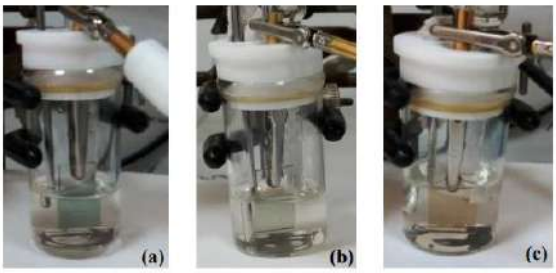


Figure 1: Colour change of PEDBP/ITO as a function of applied potential. (a) Polarized at 0.9 V. (b) Polarized at -0.2 V. (c) Polarized at -1 V.

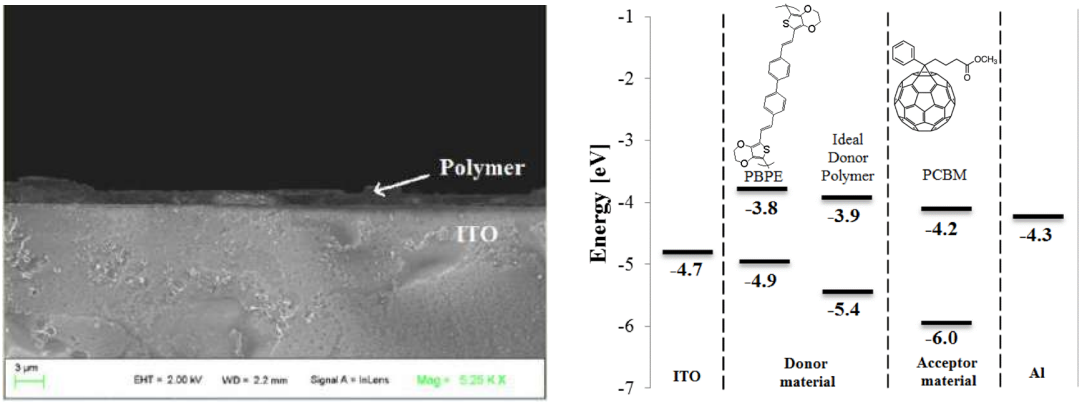


Figure 2: SEM of PBPE coated ITO - HOMO and LUMO energy levels calculated for PBPE in bilayer organic photovoltaic cells

The energy levels of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) were determined to be -4.9 eV and -3.8 eV, respectively. The optical and electrochemical band gaps were calculated as 1.08 eV and 1.49 eV. Due to its favorable electronic properties, PBPE shows potential as a donor material in organic photovoltaic solar cells when paired with PCBM as an acceptor material.

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Analysis of silver nanoparticles in pharmaceutical and biomedical products

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Nanotechnology has advanced significantly over the last decade and has found several uses in fields as diverse as medical, pharmaceuticals, microelectronics, aerospace, and the food industry (Pawar et al., 2023). Recently, there has been a growing interest in metal nanoparticles, particularly silver nanoparticles (Ag-NPs) (Magdy, 2024).

Silver nanoparticles are particles in the size ranging between 1 and 100 nm. The two major methods used for synthesis of silver nanoparticle are the physical and chemical methods with the disadvantage that they are expensive and can also have toxicity (Mathur et al., 2018)

In context of green chemistry, Ag-NPs produced by biological method are far superior compared to those manufactured with physical and chemical techniques. In the process of global efforts to reduce hazardous waste, there is always need to develop a synthesis route which is economical, cost effective, non-toxic and productive (Dhaka et al., 2023).

Biosynthesis of nanoparticles can occur in two ways-bio-reduction or biosorption. In the case of bio-reduction, the silver ions are reduced to into more stable forms biologically (Vishwanath & Negi, 2021).

This, in turn, has increased the potential for interactions of AgNPs with terrestrial and aquatic environments, as well as potential exposure and toxicity to human health.

The major routes of entry of NPs are ingestion, inhalation, dermal contact and, directly in systemic circulation via intraperitoneal (i.p.) or intravenous (i.v.) injection (Ferdous & Nemmar, 2020)

AgNPs accumulated in duodenum as first contact site and transferred to other target tissues; in liver and duodenum, they were free in the cytoplasm or included in organelles (Narciso et al., 2020)

The use of AgNPs in biomedicine has been pivotal in the creation of cutting-edge antimicrobial agents, tissue restoration and regeneration materials, biomaterial and medical device coatings, drug delivery formulations, detection and diagnosis platforms, and performance-enhanced therapeutic alternatives (Burdușel et al., 2018; Meher et al., 2024).

Reports suggest that AgNPs can induce cell death, DNA damage, and oxidative stress in various cell types. The toxic effects of AgNPs differ based on their size, shape, surface charge, and coating. The molecular mechanisms behind the toxicity of AgNPs involve the production of reactive oxygen species, disruption of cellular membranes, and activation of proinflammatory cytokines (Waktole, 2023; AlAtawi et al., 2024).

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Guidelines for abstract submission for the congress 1st-ICRAMPCS 2024

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Synthesis and Characterization of a Cobalt(III) Schiff Base Complex [CoIII(L)3]: Structure Analysis and Drug-Likeness Profiling with SwissADME

A novel Schiff base complex, formulated as [CoIII(L)3] with [HL: N'-(propan-2-ylidene)furan-2-carbohydrazide], was synthesized in-situ through the condensation reaction between hydrazide and acetone in an alcoholic solution, followed by complexation with cobalt(II) via a reflux method [1]. The synthesis resulted in the formation of a precipitate, which was recrystallized in DMF, yielding dark crystals suitable for single-crystal X-ray diffraction (XRD) analysis [1]. Characterization techniques, including XRD, confirmed the crystallization in the P-1 space group with unit cell dimensions a = 9.3480(5) Å, b = 11.0695(6) Å, c = 13.1553(7) Å, and angles α = 88.428(2)°, β = 75.774(2)°, γ = 69.227(2)°. The calculated volume (V) was 1231.07 Å³, with Z = 2 [1]. The cobalt center was oxidized to cobalt(III) during the complexation, leading to coordination by three oxygen and three nitrogen atoms from the imine groups, forming a distorted octahedral geometry [1].
FT-IR analysis revealed key absorption peaks at 1676 cm−1 (C=N stretching), 2958–2922 cm−1 (C-H stretching), and other regions corresponding to C=C and C-N stretching, confirming the presence of functional groups associated with the hydrazone structure [1]. Intramolecular contacts, such as CH..O and CH..N, indicate stability and conformation within the molecule, while intermolecular contacts, particularly CH…O, CH…N, CH…C, and Van der Waals forces, ensure interactions between different molecules that stabilize the crystal structure [1]. The complex, with a molecular weight of 557.46 g/mol, features 37 heavy atoms, 3 rotatable bonds, 6 hydrogen bond acceptors, and 3 donors. The compound exhibits moderate solubility in water (Log S -5.41 to -8.75) and demonstrates high gastrointestinal absorption but does not penetrate the blood-brain barrier [2]. Additionally, it fails to meet Lipinski's or Ghose's criteria for drug-likeness, while complying with Veber and Muegge's rules. Its synthetic accessibility score is 5.75 [2].
In conclusion, this compound shows potential as a drug candidate due to its favorable gastrointestinal absorption and moderate solubility, but its violations of key drug-likeness rules may limit its viability as an effective therapeutic agent. Further optimization may be necessary to enhance its properties for medicinal use.

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Novel Cobalt(II)-Sulfamethoxazole Complex: Structural Characterization, and Hirshfeld Surface Study

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As one of the oldest classes of antimicrobials, sulfonamides are still widely used to treat diseases such as cancer and tuberculosis [1]. They are an important group of medicinal compounds, primarily utilized as antibacterial agents by interfering with p-aminobenzoic acid (PABA) in the biosynthesis of tetrahydrofolic acid, essential for bacterial metabolism [2].

Sulfamethoxazole, a derivative of p-amino-benzene sulfonamide, contains donor groups (Ar—NH_2, NH sulfonamide, SO_2—R, and heterocyclic N, O atoms) capable of interacting with metal ions, allowing it to act as a monodentate or bidentate ligand [3].

The novel Cobalt (II) complex with the sulfamethoxazole (SMX) ligand was successfully synthesized via a conventional soft chemistry method. This was achieved by reacting cobalt acetate with sulfamethoxazole in an ethanol solution containing imidazole.

The reaction mixture was heated with continuous stirring until complete dissolution of the compounds. The resulting solution was left at room temperature, leading to the formation of purple crystals suitable for X-ray diffraction after several days.

Single-crystal X-ray diffraction data were collected at 296 K using a Bruker Apex II diffractometer. The structure was solved with SHELXS97 and refined using SHELXL97. Hydrogen atoms were mostly placed in calculated positions, with water molecule hydrogens located via Fourier maps.

The asymmetric unit of the compound consists of a cobalt atom situated on an inversion center, with an occupancy of 50%. This cobalt atom is coordinated to one molecule of sulfamethoxazole, one molecule of imidazole, and one molecule of water. The remaining portion of the structure is generated by symmetry, forming a polyhedral environment around the metal center.

The coordination environment of the cobalt atom can be described as a slightly distorted octahedral geometry, achieved through coordination with two nitrogen atoms from the imidazole group, two nitrogen atoms from the isoxazole group, and two oxygen atoms from two aqua ligands.

The crystalline cohesion of this compound is established through a three-dimensional network of moderate intra- and intermolecular hydrogen bonds, including C-H…O, O-H…N, N-H…O, and C-H…N interactions. Utilizing X-ray data, the graphical interface CrystalExplorer 3.1 allows for the classification, visualization, and quantification of these interactions within the crystal structure.

The intermolecular interactions are further analyzed by studying the Hirshfeld surface (HS) [4], which provides insight into the molecule's shape and its interaction with the surrounding crystalline environment.

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Chemical Composition of Pepper Agro-Waste Oil Extracted by Supercritical-CO2

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The responsible and effective management of agro-food waste, poses a significant challenge for manufacturers in the pepper paste industry who prioritize environmental concerns. Addressing this challenge necessitates the exploration and implementation of sustainable waste disposal practices to reduce the impact on the environment. Strategies such as reusing valuable components, and adopting eco-friendly technologies can play a crucial role in ensuring the safe and efficient disposal of pepper waste while aligning with the focus on environmental conservation objectives and circular economy practices, for this purpose the current study has encouraged the utilization of supercritical fluid extraction as an approach to extract oil from pepper waste. This method is chosen deliberately to eliminate any potential presence of organic solvents, ensuring a cleaner and green extraction process.

Carbon dioxide, operating under supercritical conditions, was selected as the preferred fluid due to numerous advantages associated with this alternative method. Supercritical extraction of oil from pepper agro-waste sample obtained from an Algerian agro-food industry was carried out at 328 K temperature, 30.0 MPa pressure and 50 g/min CO2 mass flowrate, these operating conditions resulted in an oil extraction yield of 12,25 %.

Furthermore, the qualitative analysis and the chemical composition in the crude extract were analyzed by gas chromatography coupled with mass spectrometer (GC-MS), which allowed the identification of biologically important volatile compounds, including fatty acids, Alkaloids, and hydrocarbons, but the four major ones, namely 9,12-Octadecadienoic acid (Z,Z)-, Hexadecanoic acid, Capsaicin and Dihydrocapsaicin, are present with significant percentages, showing the potential of the residual agro-food biomass as well as promoting reused resource in circular economy.

Keywords: agro-food waste, supercritical carbon dioxide extraction, green chemistry, chemical composition.

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Prediction, in silico, de l'activité anticancéreuse de nouveaux dérivés du pracinostat par inhibition des histones désacétylases

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Le benzimidazole est un composé organique hétérocyclique. Cette structure occupe une place importante en chimie médicinale et présente un intérêt considérable pour la découverte de nouveaux composés bioactifs. En particulier, ce noyau est un pharmacophore de base pour la conception de nouveaux médicaments anticancéreux.

Dans notre travail, nous nous sommes intéressés à la conception d'une série de nouvelles molécules qui sont des inhibiteurs probables de HDAC1 (5ICN). La série comprend sept composés, P1, P2, P3, P4, P5, P6 et P7, proposés en s'inspirant du pracinostat (un dérivé du benzimidazole, un inhibiteur de HDAC1). Un docking moléculaire a été réalisé pour les sept molécules de la nouvelle série avec le logiciel Autodock Vina (ADV). Une étude in silico des propriétés physicochimiques, pharmacocinétiques et de toxicité a été réalisée à l'aide des serveurs SwissADME et admetSar respectivement. Notre étude a été complétée par l'évaluation de la réactivité chimique des nouveaux proposés en faisant appel à la théorie de la fonctionnelle de la densité (DFT).

Le composé p7 a montré le meilleur score d'affinité qui est égale à -8,6 Kcal/mol comparé aux autres molécules de la nouvelle série et à la référence pracinostat avec un score de -6,6 Kcal/mol. Le complexe P7/ HDAC1 a été formé par une forte liaison hydrogène avec GLY B :97 (d=1,91 Å) et stabilisé par d'autres interactions telles que la liaison hydrogène carbone (GLY B:25), Pi-Sigma (THR A:308), Pi-Pi T-Shaped (TYR B:23), Alkyl (LEU A:320) et Pi-Alkyl (PRO B:101, TYR B:23). Le P7 a également montré un bon profil pharmacocinétique et une réactivité chimique acceptable.

Cette étude doit être complétée par une étude in vitro afin de confirmer les résultats obtenus après synthèse chimique des molécules.

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Purification of water contaminated with violet crystal dye using kaolinite composite with leftover bean peel

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Abstract:

As a promising and efficient adsorbent for the removal of crystal violet (CV) dye from aqueous solutions, a novel environmentally friendly kaolinite–cellulose (Kaol/Cel) composite was made in this study using leftover red bean peels (Pharsalus vulgaris) as a source of cellulose. By evaluating its main influencing components, the Box–Behnken design was utilized to enhance CV adsorption on the composite: loading Cel into the Kaol composite matrix (A: 0–50%), adsorbent dosage (B: 0.02–0.05 g), pH (C: 4–10), temperature (D: 30–60 ◦C), and duration (E: 5–60 min). The following significant interactions have the highest CV elimination efficiency (99.86%): The CV's maximum adsorption capacity (294.12 mg/g) was observed for BC (adsorbent dosage vs. pH) and BD (adsorbent dose vs. temperature) at optimal settings (A: 25%, B: 0.05 g, C: 10, D: 45 ◦C, and E: 17.5 min). According to these results, Kaol/Cel may be a good starting material for creating an extremely effective adsorbent that can eliminate cationic dyes from aqueous solutions.

Keywords: Environmentally Friendly, Crystal Violet, Aqueous Solutions.

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Préparation des dérivés hétérocycliques originaux de structure diversifier

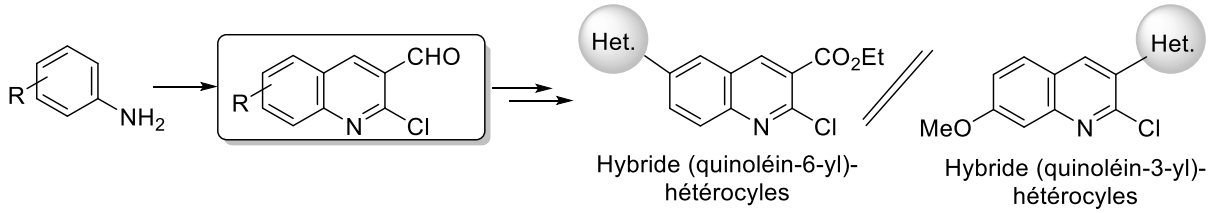
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Les hétérocycles sont des molécules importants, non seulement en raison de leur abondance et de leur extraordinaire diversité, mais surtout en raison de leur utilité aussi bien dans le domaine biologique, médicinal et autre pharmaceutique (vitamines, hormones, antibiotiques….), que technique et technologique (inhibiteurs de corrosion, colorants, agents stabilisants…). Parmi les différentes classes qui composent la famille des hétérocycles, la quinoléine et ses dérivés, qui représentent une classe importante de composés qu'on retrouve dans une grande variété de composés bioactifs naturels, et aussi dans les produits synthétiques qui ont montré une efficacité remarquable comme bactéricides, anti-inflammatoires, antalgiques, antibiotiques, anti-cancer, antihypertenseurs, et anti-VIH-1…

Cela nous a permis d'acquérir un certain savoir-faire dans le domaine, qui s'est traduit par la synthèse de bon nombre de dérivés quinoléiques nouveaux, dont certains ont montré des activités biologique remarquable (antibactériens, antioxydants anti-tumoraux et anti Alzheimer). Dans le même contexte plusieurs études ont montré que la nature et la position des substituants sur le noyau quinolyle peuvent avoir un impact considérable sur l'activité pharmacologique. Notre objectif est de préparer de nouvelles structures comportant le noyau quinolyle associé en position 6 et 3 à des hétérocycles de structures diverses. Pour cela nous avons synthétisé un certain nombre de dérivés quinoléiques originaux et pour ce faire, l'intermédiaire-clé doit présenter dans sa structure une fonction aldéhyde libre dans la position choisie.



Mots clés: Quinoléine, hétérocycle, protection, oxydation, les conditions de Knoevenagel.

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Évaluation des Effets de l'Extrait d'Althaea officinalis sur le Traitement des Lésions Gastriques Induites chez un Modèle Animal : Étude in Vivo

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Résumé

Introduction : Les lésions gastriques représentent une problématique de santé majeure, souvent causées par des facteurs comme l'infection à *Helicobacter pylori*, le stress et l'utilisation de médicaments anti-inflammatoires non stéroïdiens (AINS). *Althaea officinalis* (guimauve), reconnue pour ses propriétés médicinales, pourrait offrir une solution gastroprotectrice. Cette étude vise à évaluer l'effet de l'extrait d'*Althaea officinalis* sur la guérison des lésions gastriques induites chez un modèle animal.
Matériel et Méthodes : L'étude a été réalisée sur des rats Wistar, répartis en quatre groupes : un groupe témoin, un groupe traité avec un AINS pour induire des lésions, un groupe traité avec l'extrait d'Althaea officinalis à une dose de 200 mg/kg/jour, et un groupe traité avec un médicament anti-ulcéreux standard. Les lésions ont été induites par administration d'AINS pendant sept jours. L'extrait de plante a été administré par voie orale pendant 14 jours. L'évaluation des lésions a été réalisée par observation macroscopique et histologique.
Résultats : Les résultats ont montré que le groupe traité avec l'extrait d'*Althaea officinalis* a présenté une réduction significative du diamètre des lésions par rapport au groupe témoin ($p < 0,05$). L'analyse histologique a révélé une amélioration de la structure gastrique, avec une diminution de l'inflammation et une augmentation de la régénération cellulaire. Les résultats du groupe traité avec le médicament anti-ulcéreux standard étaient comparables à ceux du groupe traité avec la guimauve.
Discussion : Les résultats indiquent que l'extrait d'*Althaea officinalis* possède des propriétés gastroprotectrices. Les mécanismes sous-jacents pourraient inclure des effets anti-inflammatoires et mucoprotecteurs. Comparativement aux traitements conventionnels, l'utilisation de la guimauve pourrait offrir une alternative naturelle dans la gestion des lésions gastriques.
Conclusion : L'extrait d'*Althaea officinalis* démontre un potentiel significatif dans le traitement des lésions gastriques induites. Des études complémentaires sont nécessaires pour isoler les composés actifs et clarifier les mécanismes d'action.

Keywords: lésion gastrique, extrait d'*Althaea officinalis*, étude in vivo, gastroprotection

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Fagonia Bruguieri D.C Phytochemicals: review article

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Abstract

Fagonia Bruguieri (zygophylaceaes) a medicinal plant commonly used in traditional medical prescriptions in the Indian subcontinent and North Africa, where local residents claim that this plant is useful in treating some diseases such as liver and digestive system diseases. In addition some laboratory studies proved that this plant has several biological activities as an anti-inflammatory and antioxidant. In order to develop an effective medical treatment against the previously mentioned diseases, the chemical composition of the plant must be determined and compounds with biological activity identified. This is what we seek in this study by collecting previous literature that was able to identify part of the components of this medicinal plant in the Google Scholar search base. By using specific keywords in Google scholar database studies about the Fagonia Bruguieri chemical composition have been collected. The results showed that this plant is rich in Phytochemicals: Phenol, alkaloids, flavonoids, terpenoids, saponin, diterpenes of erythroxan-type cardiac glycosides, and Flavonol glycosides. In addition, the chemical composition of twenty-eight chemical compounds found in this medicinal plant was determined, two of which were discovered for the first time. Although some chemical compounds of this plant have been identified, compounds with biological activity have not been identified, and therefore there is an urgent need for more research on its chemical composition.

Keywords: Fagonia Bruguieri; Medicinal plants; Phytochemicals; review article

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Comparative study of the photodegradation of two reactive dyes.

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Environmental pollution is an issue of global concern. It is, in fact, a consequence of the rapid industrialization in many countries and the massive use of synthetic organic compounds (such as pesticides, dyes, etc.) as well as inorganic compounds (metals and non-metals). Dyes, particularly those resulting from discharges of the textile industry into aquatic environments, can have a highly detrimental impact on these ecosystems, potentially leading to the systematic destruction of fauna and flora

In this work, we focused on two Advanced Oxidation Processes : UV_{254nm}/H_2O and UV_{254nm}/acétone. To verify the effectiveness of these systems in the removal of Reactive Red 184 and Reactive Orange 4, a kinetic approach was studied. Initially, the study focused on the transformation of the dyes under direct excitation (λ=254 nm). This process strongly depends on the dye concentration: low concentrations (< 0.05 mM) lead to significant degradation rates, while the kinetics remain slow for higher concentrations (> 0.05 mM).

In the second phase, we focused on the transformation of dyes induced by the excitation of acetone and hydrogen peroxide at λ = 254 nm. These processes significantly accelerate dye degradation, which increases with higher initial doses of H_2O_2 and acetone. The acetone/UV system was more efficient than the UV/H_2O_2 system, and the order of reactivity was consistently RO4 > RR184, regardless of the initial concentration. Radical identification tests revealed the involvement of •OH and •CH3 radicals (> 80%) in the UV/H_2O_2 and UV/acetone processes, respectively. A thorough comparison of the phototransformation rates of different processes applied to various dyes was conducted to establish a ranking of reactivity, both for the processes used and for the dyes.

Keywords : *Photooxidation, Dye, Comparison, Kinetics, Operating Factors.*

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Advances in nanostructured catalyst for enhanced organic synthesis: innovations and applications

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Transition metal phosphates have been the subject of numerous studies. Among these materials, iron phosphates have attracted particular interest due to their electrochemical properties, compositions, and activities. This material is known as an electrode and a catalyst for oxidation reactions**[1].**

In this work, we studied a new synthesis route to prepare pure iron(III) phosphate (FePO4). The preparation method of the catalyst is key to its structure and activity**[2].** FePO4 is synthesized from aqueous solutions using urea. The obtained material was characterized by various techniques such as FTIR spectroscopy, X-ray diffraction (XRD), UV-VIS spectroscopy, BET analysis, and Raman spectroscopy.

The use of our material remains limited in organic synthesis compared to other heterogeneous catalysts, particularly in the C-C coupling reaction for the synthesis of propargylamines, which are important intermediates for the synthesis of drugs and heterocyclic molecules**[3].** The catalyst demonstrated high activity in the synthesis of propargylamines via the A3 coupling of amine, aldehyde, and alkyne.

We concluded that FePO4 reduced the reaction time to 4 hours with great stability and good yields ranging from 70% to 98%

Keywords : Heterogeneous catalyst, A3 coupling, FePO4, Transition metal, Propargylamine synthesis, Hydrothermal route.

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Synthesis and physicochemical characterization of pure and Al doped TiO_2 photocatalysts

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Abstract

Pure and doped titanium dioxide (TiO_2) nanostructures with aluminium at different percentages (0.2%, 0.5%, 1% and 1.5%) are successfully elaborated by the sol-gel process under the supercritical conditions of isopropanol and then calcined at 600°C for one hour.

The obtained powders are characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM).

XRD analysis showed that the rutile phase is the predominant phase in pure TiO_2 and the doping with aluminium led to the decrease in peak intensity and the appearance of some peaks of the anatase phase for a doping concentration of 1.5%, while no diffraction peak due to Al metal appeared, suggesting that the metal particles are well dispersed on the TiO_2 surface or are present in too small quantities.

IR spectroscopy detected the presence of hydroxyls that promote the photocatalysis reaction, it highlighted TiO_2 products such as the presence of bands in the 400–800 cm^{-1} region which can be attributed to the vibration modes of Ti - O and Ti - O - Ti bands.

The surface morphology of pure TiO_2 and TiO_2-Al calcined for one hour at 600°C was studied using SEM and EDX analysis. These analyses show that the powders examined are composed of aggregates of large particles and porous morphology, this is probably due to the adopted synthesis method (sol-gel) and the nature of the precursors used (titanium isopropoxide and aluminium nitrate). These catalysts do not have uniform microstructure, but few pores are formed in the pure TiO_2 photocatalyst compared to the Al-doped photocatalysts. On the other hand, the results obtained show that the aggregates in TiO_2-Al are larger than in pure TiO_2. This means that the addition of Al is effective in modifying the morphology of TiO_2. Moreover, cracks on the surface of the photocatalysts are observed, which may be due to the shrinkage of the samples caused by phase crystallization during the calcination process.

Furthermore, the corresponding EDX spectra of pure and Al-doped TiO_2 powders indicate the presence of Ti, O and Al confirming the purity of the prepared samples. In addition to this, a very weak signal for Al compared to the very strong signal for Ti, signifies the agreement with the expected molar ratios of each sample with the starting stoichiometry.

These TiO_2 nanostructures were elaborated for application in the elimination of organic pollutants by photocatalysis.

Keywords: TiO_2, aluminium, doping, photocatalysts, pollution.

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Nitrate and nitrite quantification in animal Product marketed in Algeria

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Perceived global changes in eating habits emerge as a major concern of the 21st century [1]. Face to the development of the agri-food industry, North Africa is no exception to these changes [2].

The addition of nitrites and nitrates as food additives in the manufacturing of animal products, such as processed meats, is a common and essential practice for industry due to their advantageous technological versatility. However, this use remains concerning regarding its impact on consumers health.

Our study focused on evaluating the concentrations of nitrites and nitrates in meat products sold in the wilaya of Tizi-Ouzou (Algeria). We analysed 30 samples using two distinct determinations via UV-visible spectrophotometry for each sample. After deproteinization, nitrites were measured using the reference colorimetric method with N-naphtylethylenediamine [2], while nitrates were quantified using the sodium salicylate method.

Additionally, a descriptive study was conducted to identify and categorize different additives based on their role and frequency of use. The results revealed that 100 % of the analysed products contained nitrite concentrations below the authorized standard, whereas 70 % exceeded the regulatory limit for nitrates. Furthermore, the descriptive analysis identified a significant number of additional additives.

This article highlights observed irregularities and potential risks associated with consuming such products, while also suggesting potential alternatives to preserve consumers health.

Keywords: Nitrites, Nitrates, Meat products, Food additives, Assay.

References:

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Caractérisation et Étude cristallographique du 1-[4-({4-[(E)-(2-Hydroxynaphthalen-1- yl)methyl ideneamino] phenyl} sulfanyl)-phenyl]ethenone

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Dans cette étude ont présenté la caractérisation structurale d'une bases de Schiff soufrées à partir de 4-amino-4'-acetyl-diphenylsulfide le 1-[4-({4-[(E)-(2-Hydroxynaphthalen-1-yl)methylideneamino] phenyl} sulfanyl)-phenyl]ethenone cristallise dans le système monoclinique, Son groupe d'espace est Cc sous la forme phénol-imine. [1]

Cette forme est favorisée par une forte liaison hydrogène intramoléculaire O-H…N, et adopte une conformation E autour de la liaison C═N. La structure est stabilisée par quatre liaisons hydrogène intermoléculaires de types de C-H··· O. Dans la structure cristalline, les molécules sont alignées tête-queue le long de l'axe b [2]

Cette étude a été consolidée par une analyse de la surface Hirshfeld. : L' analyses de la (SH), montre des interactions moléculaires spécifiques, mettant en lumière un empilement π-π remarquable pour ce composé. [3]

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Corrosion inhibition of titanium by propolis in fluoride saliva: An electrochemical analysis

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Abstract :

Titanium and its alloys, such as Ti-6Al-4V, are commonly used as implant materials, including dental and orthopedic implants [1,2], due to their high corrosion resistance in physiological environments, low toxicity, and excellent biocompatibility [3,4]. Commercially pure titanium (cp-Ti) has been widely used in dentistry for many years in the production of crowns, bridges, and other devices [3].

The aim of this study was to investigate the effect of fluoride and propolis extract on the corrosion behavior of commercially pure titanium (cp-Ti grade 2) in artificial saliva. Corrosion inhibition studies were conducted on cp-Ti, used as a dental implant, in Fusayama-Meyer artificial saliva with the addition of propolis extract, utilizing potentiodynamic polarization and Electrochemical Impedance Spectroscopy (EIS). Variables such as inhibitor concentration and immersion time were adjusted and optimized. The results indicated that both the presence of NaF and propolis extract in the saliva significantly affected the corrosion rate (I_{corr}) and polarization resistance (R_p). The I_{corr} increased and R_p decreased in the fluoride-containing medium, whereas the addition of propolis improved the corrosion resistance of the titanium.

Keywords-Propolis; Titanium grade 2; Inhibition; Fusayama-Meyer; Electrochemical Impedance Spectroscopy

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Antioxidant activity and chemical composition of *Centaurea* genus essential oil

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Aromatic plants are often used as natural remedies due to their inherent corrective and pharmacological properties. The study of natural resources, especially products of plant origin, has become an exciting field of research for the discovery and development of drugs. Aromatic plants are mainly exploited for the extraction of essential oils for industrial applications, such as cosmetics, flavoring and fragrance, spices, pesticides, repellents and herbal drinks [1].

A large number of these aromatic plants belong to the Asteraceae family, one of the largest families of flowering plants, comprising over 1600 genera and 25,000 species worldwide [2], many of which produce essential oils used in folk and modern medicine.

Centaurea is one of the most important genera in this family, contains approximately 700 species distributed all over the world [3]. In Algeria, it is represented by 45 species, seven of which occur in the Sahara Desert [4].

The aim of this study was to identify the chemical composition of essential oil of *Centaurea* genus by GC/MS analysis and to compare the results to bibliographic data in the world as well as the identification of the geographical distribution of chemotypes in Algeria. The aerial parts of *Centaurea* genus were subjected to hydro-distillation in a Kaiser Lang apparatus, the oil obtained was analysed by GC-MS. As a result, thirty -five compounds, accounting for 94.28% of the total oil, were identified. The major constituents of the oil were docosane-11-decyl (15.98%), dodecanoic acid (7.93%), (-) Spathulenol (7.44%), (-) caryophyllene oxide (5.38%), α-pinene (4.05%), 6,9,12-octadecatrenoic acid, methyl ester

(3,72%) and dotriacontane (3.66%). Furthermore, the essential oil was screened for their antioxidant activity using DPPH method. The result indicate that the essential oil has low activity compared to the reference antioxidant compounds.

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In vitro anti-inflammatory, antioxidant, and antibacterial activities of *n*-Butanol Extract from Indigenous Algerian *Ficus*

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Exploring natural products for their potential health benefits has increased interest in the phytochemical properties of various species extracts. This study investigates the antibacterial, anti-inflammatory and antioxidant activities of the *n*-butanol extract from an endemic Algerian *ficus*, prepared from the dried *ficus* plant and subjected to various in vitro assays to evaluate its biological activities[1].

The antibacterial activity they assessed using the well-diffusion method in DMSO, against a panel of gram-positive and three gram-negative bacteria, including *Staphylococcus aureus*, *Escherichia coli*, *Morganelle morganii*, and *Pseudomonas aeruginosa*. The extract demonstrated significant antibacterial activity, particularly against *Pseudomonas aeruginosa and Escherichia coli*.

The membrane stabilizing activity of *n*-butanol extract was evaluated by using hypotonic solution-induced human erythrocyte hemolysis[2], and the results showed a 100% inhibition at 3 mg/mL and 2mg/ml in comparison with 96.54 ± 2.14% observed with diclofenac in tested doses.

The Antioxidant activity was evaluated using a DPPH (2, 2-diphenyl-1-picrylhydrazyl) radical scavenging assay[3]. The *n*-butanol extract exhibited strong DPPH radical scavenging activity with 84.13% at 0.5 mg/ml with an IC50 value of 0.218 mg/ml, indicating its potential as a natural antioxidant.

The results suggest that the *n*-butanol extract from *ficus species possesses* potent anti-inflammatory and antioxidant properties, making it a promising candidate for further development in pharmaceutical and nutraceutical applications.

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Design, characterization and application of complexes based on of heterocyclic ligands : nitrogenous

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In molecular chemistry, a complex is defined as a polyatomic structure composed of one or more metal cations surrounded by several ligands. The term ligand is used to describe molecules or ions that delocalize part of their electron density to a cation and form chemical bonds with this cation, called coordination bonds. [1,2].

Our research team has recently developed a research axis devoted exclusively to imidazole derivatives (synthesis, characterization and application) [3]. Based on our experience in the field, we have explored the behavior of compounds capable of competing in dynamic fields such as the chemical, pharmaceutical, biomedical, agri-food, phyto and biosanitary industries, as well as in the production of new materials, in environmental control, in analysis and quality control, and in the field of renewable energies

In this work we will present the preparation, the characterization and the structural description of the results to which we have reached during the various complexation reactions between ligands containing (imidazole) as base nucleus, previously prepared, and the metal salt, and a new coordination complex based on this ligand of general formula [M(II)L1 or 2Cl2].The complex were obtained by the action of ligands on metal salts in a metal salt /ligand ratio. the complex were characterized by X-ray diffraction on single crystal and on powder, NMR, IR and UV-vis spectroscopy analysis. The study of the hydrogen bond network and the analysis of the Hirsfeld surface .as well as the analysis, the stability of the prepared ZnII complexes was evaluated using the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), and the energy gap. The molecular geometries and the electronic transitions of the two complexes and their ligands in the ground state have been calculated using the mPW1PW91 base at the theoretical level TZVP [5]. have been realized

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Bis-isoQuinolinium Salts Derivatives as inhibitors for mild steel corrosion in acid media: Thermodynamic, electrochemical and quantum chemical evaluation.

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Mild steel is widely used in a variety of industrial applications such as petroleum industries, power plants, etc. Sulfuric acid solutions are widely used for pickling, descaling, acid cleaning, oil-well acidizing, etc. The use of inhibitor is one of the best known methods of corrosion protection. The efficiency of inhibitor depends on the nature of environment, nature of metal surface and electrochemical potential at the interface, and the structural feature of inhibitor, which includes number of adsorption centres in the molecule, their charge density, the molecular size, and mode of adsorption, formation of metallic complexes and the projected area of inhibitor on the metal surface [1].

Organic compounds containing hetero-atoms such as N, O and S have been reported efficient corrosion inhibitors for metals and alloys [2]. In acidic environments, organic compounds with more than one hetero-atoms containing pi-electrons exhibit high inhibiting properties by providing electrons to interact with metal surface [3]. It was also found that the protection efficiency was also found to be improved by increasing the length of the alkyl chain and the organic compound concentration.

In our previous works, we have focused on heterocyclic derivatives as inhibitors against the acid corrosion of steel [4]. In continuation, this work aims to evaluate the inhibition efficiencies of two bis-isoQuinolinium salts on A283 Grade C mild steel corrosion in a 0.5M H_2SO_4 medium. The studied inhibitors have two iso-Quinolinium groups and a linear chain hydrocarbon in their structures. electrochemical impedance spectroscopy, weight loss experiments, and potentiodynamic polarization measurements were all used in this study. We also examine the performance of corrosion inhibition by studying the influence of temperature on the corrosion process. Density functional theory (DFT) is used to investigate the relationship between electronic structure of inhibitors and experimental inhibition efficiencies.

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DFT and experiment study on adsorption of heavy metals using a low cost activated carbon prepared from local biomass

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Despite advancements in technology and the implementation of stricter environmental regulations, pollution from industrial activities has continued to escalate, contributing to the ongoing deterioration of water quality [1]. Industrial wastewater, often laden with hazardous heavy metals such as nickel, copper, lead, cadmium, and zinc, represents a serious threat to both human health and ecosystems. Over the past three decades, there has been significant scientific interest in exploring the mechanisms and effectiveness of heavy metal adsorption in aquatic environments, with the goal of mitigating their harmful impact on water resources [2-4].

Consequently, this study focused on the removal of copper and chromium from water by utilizing low-cost activated carbon derived from chestnut shells. The equilibrium data aligned most closely with the Langmuir isotherm model, indicating that this model effectively describes the adsorption process. The maximum adsorption capacities (qm) for Cu(II) and Cr(VI) ions, as calculated from the Langmuir model, were 33.33 mg/g and 26.79 mg/g, respectively. These values suggest that the activated carbon demonstrates a stronger adsorption capacity for Cu(II) compared to Cr(VI), although the initial interpretation may indicate a higher affinity for copper. However, the higher qm value for Cu(II) reflects its greater overall adsorption potential on the activated carbon surface.

A theoretical study employing Gaussian 09 software and Density Functional Theory (DFT) was carried out to investigate the formation of organometallic complexes between

functionalized activated carbon and metal ions [5-6]. The adsorption of these metal ions was influenced by the carboxyl and amine groups present in the activated carbon derived from chestnut shells (CNS-AC). The calculated bonding energies for copper and chromium with the adsorbent were found to be 1163.303 kcal/mol and 1160.713 kcal/mol, respectively. Comparing these values revealed that copper forms a stronger bond with the activated carbon than chromium, indicating a higher affinity of the adsorbent for copper. The proposed new model and DFT investigation explained well the involved functional groups in the targeted heavy metal ions uptake by CNS-AC. Furthermore, a good agreement between experimental and theoretical approaches was observed.

Keywords:

Adsorption; Heavy Metals; Activated Carbon; DFT; Water treatment.

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LEAD SQUARATE POLYMORPH

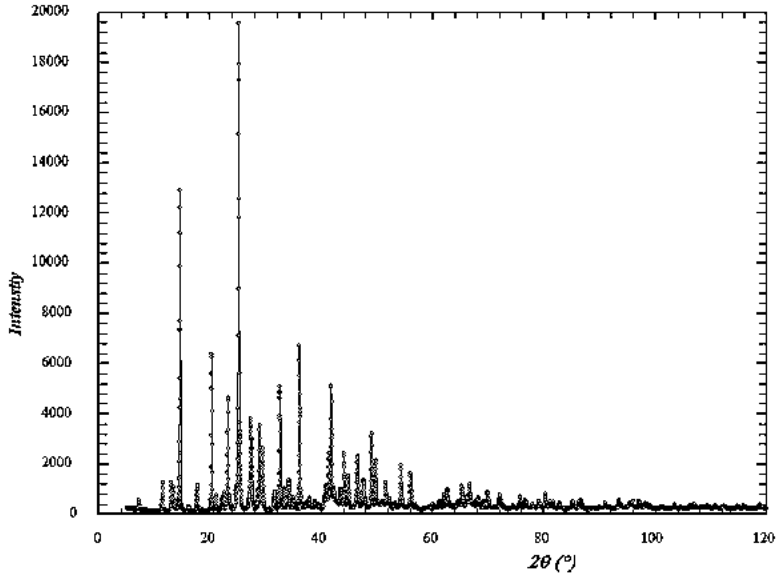
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Starting from $Pb(H_2O)_4(C_4O_4)$, powder data of Lead squarate polymorph were collected in air at 140 °C with a Bruker AXS D5005 diffractometer using a diffracted-beam-graphite monochromator (Cu $Ka_{1,2}$) and equipped with a Anton Paar HTK1200 oven camera.

The pattern was scanned at room temperature, over the angular range 5–120° (2*θ)*, with a step length of 0.02° (2*θ)*. Powder pattern indexing was performed with the program DICVOL04, leading to the orthorhombic unit cell: a = 24.268(4) Å, b = 15.270(3) Å, c = 7.854(1) Å et V = 2910.6 Å^3, Z = 4 [M_{20} = 26, F_{25} = 48 (0,0053;98)]. The systematic absences revealed by a careful examination of the powder data are consistent with the space group *Cmma*.



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Preparation and characterization of Titanium Dioxide and Alumina supported on Montmorillonite and theirs application in remediating of Basic Fuchsin by adsorption.

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Abstract

Our work focuses on the intercalation (impregnation) of montmorillonite-type clay (K10) with 10% titanium aluminum oxide, with the aim of improving the catalytic properties of montmorillonite. DRX analysis shows a de-lamellarized structure of both prepared catalysts. FT-IR analysis shows the presence of characteristic bands of clay, Tinium oxide and Alumina. These materials have been used for the decontamination of Basic Fuchsin (BF). TiO_2 nanoparticles supported by montmorillonite demonstrated superior decontamination efficiency against FB. They chemically degraded 98.83% of BF in 2 hours, compared with 94.26% FB removal over 3 hours for Al- MT. Bare montmorillonite showed the lowest decontamination efficiency of all materials against FB. It decontaminated only 90% of FB in 4 hours.

Keywords: Impregnation, montmorillonite, titanium oxide, Basic Fuchsine, Adsorption.

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Preparation of Ceramic microfiltration membranes using for wastewater treatment

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Abstract

Ceramic membraneshave specific properties, such as long-term stability at high temperatures, resistance to high pressure drops [1, 2], which attracted the attention of many academics and researchers of applied sciences in recent years [3, 4].
In this work, we prepare a ceramic microfiltration membranes using for wastewater treatment. The supports were prepared by using the quartz Sand and Calcite as starting materials. These powders were mixed with certain organic additives to obtain a conveyable paste used to prepare membrane supports with tubular configuration by the extrusion method. Afterward, the prepared supports were sintered at 1250 °C for 1 hour. These supports have good characteristics, such as high porosity ratio (45%), compression strength (about 15 Mpa), and homogenous surface morphologies. Then, the quartz sand powder was used to prepare an intermediate membrane by using a slip casting method, after that this membrane was sintered at 1200 °C. Moreover, the top-layer Zircon ($ZrSiO_2$) membrane was performed by the same method and sintered at 1190 °C. The obtained results showed that this membrane has a high permeability value of distilled water (about 480 $l.h^{-1}.m^{-2}.bar^{-1}$), high efficiency to remove the heavy metals such as (Fe (78%), Al (60%), Zn (53%))…….etc , and a good rejection performance of methylene blue (75%).
As a conclusion, the results indicated that this top-layer membrane is suitable for some microfiltration applications, especially for wastewater treatment.

Keywords: Quartz Sand, Zircon, Supports, Membranes, Microfiltration.

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Application of a green emulsion liquid membrane prepared from vegetable oil for water decolourisation: Process optimisation using response surface methodology.

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Liquid emulsion membrane (ELM) technology is a new cost-effective and energy-efficient technique for extracting a wide range of toxic pollutants, but the use of volatile organic solvents in the membrane phase is problematic as it directly affects the environment on several levels. To solve this problem, a new advanced and innovative Green Emulsion Liquid Membrane (GELM) process, using vegetable oils as green solvents instead of volatile organic solvents in the membrane phase, has been introduced for the treatment of coloured wastewater .

A series of experiments was carried out to study the effectiveness of different parameters on the efficiency of dye extraction from GELM using the Box-Behnken design. The aim of this research was to optimise the variables influencing the emulsified green liquid membrane technique for extracting cationic dye mixtures from an aqueous solution. The membrane used in this study comprises an organic phase and an aqueous phase.

Span80 and vegetable oil are the components of the organic phase, while H_2SO_4 represents the aqueous phase. The effects of various factors are studied, such as: the concentration of the internal phase $[H_2SO_4]_{int,}$ the volume ratio$_{Vext/Vem}$ and the mass concentration of Span80. The parameters set during the mixed extraction are: t_{em}=30s, t_{ext}=1h, O/A=2, V_{ext}/V_{em}=5, v=250tr/min, $[MG]_0/[Rh\text{-}B]_0$=1.

The results of the optimisation give a concentration of sulphuric acid used as the internal phase of 0.05M, a percentage of surfactant span80 =6% by mass and a volume ratio Vext/Vem =5, with a theoretical yield of **100%** and an experimental yield of **98.18%.**

Keywords: Extraction, GELM, cationic dye, green diluent, depollution.

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Low-Cost Bioadsorbents for Targeted Water Pollutant Removal

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Low-cost adsorbents have emerged as a promising alternative to conventional water treatment technologies for the removal of various pollutants, including heavy metals, dyes, and pharmaceutical contaminants. These adsorbents, such as eggshells and biomass-derived activated carbon, have demonstrated remarkable removal capabilities for a wide range of pollutants [1]. The adsorption process utilizing these low-cost materials is distinguished by its efficiency, operational simplicity, and reduced environmental impact, avoiding issues related to residual sludge generation.

Eggshells, in particular, have been the subject of extensive studies as a promising adsorbent, due to their abundance as waste from the egg processing industry [2]. Similarly, biomass-derived adsorbents, including biochar and activated carbon, have demonstrated significant efficacy in water treatment [3].

It is particularly noteworthy that the adsorption efficiency of bioadsorbents can be considerably enhanced through various modification techniques, such as chemical or physical activation, and functionalization [4]. These modifications optimize the structural and chemical properties of bioadsorbents, thereby rendering them more effective in removing contaminants from aqueous solutions. These materials engineering approach opens new perspectives for the development of highly efficient adsorbents specific to certain pollutants.

Keywords: Low-cost adsorbents; Adsorption; pollutants; Wastewater.

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Removal of methylene blue from aqueous solution by adsorption onto Ain Barbar feldspar

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The discharge of dyestuff industries constitutes enormous nuisance for the environment and for the human health. Therefore, the use of local clays in the treatment of the discharge has an important economic and environmental interest and with the aim for value the local's clays from Algerian East: Ain Barbar feldspar in cationic dyes adsorption, which are difficult to adsorb and frequently encountered in industries: methylene blue. Analysis of feldspar shows that silica and alumina are the majority compounds [1]. The modification of clay enhances the textural and structural properties in the adsorption of methylene blue. Optimisation of physicochemical conditions (pH, temperature, size, the type and the nature of clays) is performed in this study. Feldspar has a good adsorption capacity. The adsorption capacity was determined using the Langmuir and Freundlich isotherms. The monolayer adsorption capacity for methylene blue of purified feldspar was better than the crude feldspar. The adsorption kinetics of methylene blue were studied using the equations of the pseudo-first-order, pseudo-second-order reactions and intraparticle diffusion equation. The study of the thermodynamic adsorption parameters shows that the adsorption process of methylene blue by modified clay is endothermic, spontaneous and have a physical nature.

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Enhancing xanthate adsorption on galena during the flotation

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Abstract:

Galena (PbS) is a major source of plomb metal. It usually coexists with other sulfide minerals such as chalcopyrite, sphaletite and pyrite. Its concentration is accomplished by adsorption using short-chain thiol collectors such as xanthate "KEX". Due to its unique chemical and structural characteristics, the concentration of galena by adsorption requires activation, which is a process of making the mineral susceptible to reactions with the thiol collectors.

The activation of galena and the subsequent adsorption of potassium ethyl xanthate collectors on the surface are controlled by FTIR spectra and SEM have been used to identify the mechanism of interaction between sulphite and galena surfaces.

Activated galena with copper sulfate (10^{-4}M) has been investigated at pH 9 and potassium ethyl xanthate (3.10^{-3}M) concentration. [1]

Adsorbed colloidal (Pb-EX, 1123.08Cm^{-1}) is found even at high xanthate concentration, colloidal lead oxide/hydroxide particles have been imaged after 10^{-4}M lead sulfate addition at pH 9.

The behaviour of this system is consistent with ion exchange between potassium ethyl xanthate and hydroxide followed by oxidation to dixanthogen (X_2, 1273.561Cm^{-1}) and diffusion of this species across the surface. [2-3]

Keywords: Xanthate (KEX), Galena, Adsorption, FTIR, SEM

1. Introduction:

Among the processes that have attracted great attention from researchers during the industrial growth that required considerable quantities of metals is the process of processing ores by flotation, which is considered the main physicochemical separation technique currently used in the mining industry. It makes it possible to separate the recoverable elements of an ore from their gangue, when the simplest and least expensive methods are not applicable

2. 1/ Qualitative determination of the adsorption of potassium ethyl xanthate (KEX) by infra-red spectroscopy:

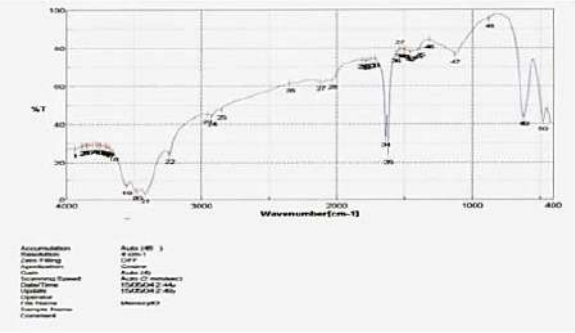


Fig. 1. Spectra FTIR of galena treated by KEX

2.2/ Qualitative determination of the adsorption of xanthate (KEX) by electron microscope with sweeping

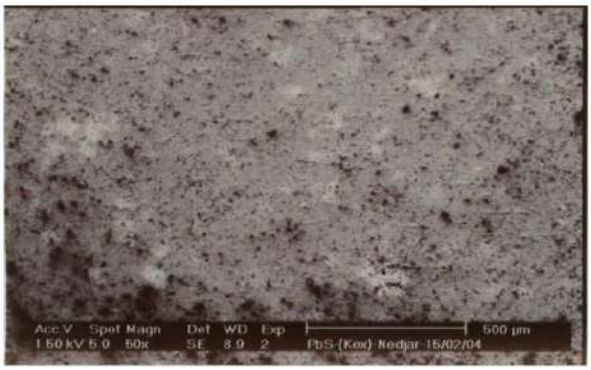


Fig. 2. Microphotography taken with the electron microscope with sweeping (X1480):galena treated by KEX

General summary : This work allowed us to determine the extent of adsorption of potassium ethyl xanthate on the mineral surface of Galena under flotation conditions of an anionic complex of the potassium ethyl xanthate (KEX)
Galena activation and subsequent adsorption of potassium ethyl xanthate complexes on the surface were carried out by FTIR spectra, and SEM was used to determine the interaction mechanism between sulfite and galena surfaces. [4-5]

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Bulbs plant from *Asparagaceae* family as novel source of natural sunscreen and antioxidant agents

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The application of sunscreens is essential, particularly in regions with elevated ultraviolet (UV) radiation; however, natural compounds have recently been recognized as viable sunscreen choices due to their UV absorption properties and antioxidant efficacy (Ebrahimzadeh, Enayatifard et al. 2014).

The current investigation provide that bulbs plant from Asparagaceae family could be novel source of phenolic contents as photoprotective agents with strong antioxidants proprieties where methanol, dichloromethane, ethyl acetate and butanol extracts had high sun protection factor according to Commission Recommendation 2006/647/EC (Communities. 2006) comparing to commercial sunscreens Nevia and Vichy with strong superoxide anion scavenging in the same extracts. The importance results of ethyl acetate extract encouraged to separate three compounds could be responsible to these activities using chromatographic methods while will identify them using spectrophotometric methods.

Keywords: antioxidant activity, photoprotection, separation, identification.

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Electrochemical, Theoretical Studies of Corrosion Inhibition Effect of Amino Acids Compounds as Green Inhibitor for Carbon Steel in 1M HCl

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Abstract

The employment of inhibitors is one of the most effective methods for the protection of metals against corrosion. Although most synthetic corrosion inhibitors are highly efficient in acidic environments, they are expensive and pose health and ecological risks. Therefore, due to the hazardous environmental effects of synthetic inhibitors the researchers' attention has been drawn towards finding cheaper and non-toxic inhibitors [1]. In this regard, green corrosion inhibitors have recently attracted the consideration of researchers. Amino acids have captured renewed interest in corrosion inhibition. They are environmentally friendly compounds, readily available, non-toxic, biodegradable, completely soluble in aqueous media, and produced with high purity at low cost [2,3].

In this study, Amino acids: Arginine and Serine were tested as green corrosion inhibitors for X70 carbon steel in 1M HCl by using potentiodynamic polarization and electrochemical impedance spectroscopy (EIS). The results indicate that the inhibition efficiency increased with increasing concentrations. Polarization measurements showed that Arginine and Serine acted as mixed inhibitors and they were adsorbed on the steel surface following Langmuir adsorption isotherm. Moreover, Quantum chemical parameters obtained using the density functional theory (DFT) corroborated the experimental results.

Keywords: Steel Corrosion, green inhibitor, Amino acids, EIS, DFT.

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Etude gravimétrique et électrochimique du processus d'inhibition de la corrosion du zinc en milieu acide par des substances naturelles

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La corrosion représente un sérieux problème dans de nombreux domaines industriels tels que les industries pétrolières, chimiques, électriques, nucléaires, et agroalimentaire. Elle provoque des conséquences non désirées comme remplacement de pièces corrodées, arrêt de production et même risques de pollution. Ainsi, elle induit à des pertes économiques importantes allant à 2.5 billions de dollars dans le monde.

Actuellement, la protection contre la corrosion est devenue une priorité. Plusieurs méthodes sont adoptées tels que : les traitements de surface par revêtement métallique ou polymérique, la protection cathodique ou bien la modification du milieu corrosif par l'ajout d'inhibiteurs de corrosion. Ce dernier est en effet le moyen le plus original pour lutter contre la corrosion car ces substances ajoutées à faibles concentrations dans le milieu corrosif diminuent et parfois empêchent carrément la corrosion du métal [1].

Les inhibiteurs ne sont pas des substances innocentes ; elles sont toxiques et néfastes pour l'environnement, en particulier les chromates et les organophosphorés, ce qui a rendu leur utilisation limitée. Le remplacement de ces inhibiteurs par des substances non toxiques et naturelles reste la meilleur alternative [2].

L'objectif de notre travail consiste à étudier l'effet d'un inhibiteur vert préparé à partir d'une plante appartenant à la famille des moracées sur la corrosion du zinc dans une solution d'acide sulfurique.

L'étude a été réalisée en faisant appel aux techniques gravimétrique et électrochimique. Les résultats ont montré que l'efficacité de l'inhibition augmente avec l'augmentation de la concentration de l'inhibiteur atteignant 95% à 1000ppm, et que l'augmentation de la température entraine une diminution significative de l'efficacité inhibitrice. L'inhibiteur étudié devient plus performant en présence des ions bromures ou iodures.

Mot clés :

Corrosion, inhibiteur, milieu corrosif, techniques gravimétrique et électrochimique, synergie.

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Regioselective oxidative & Tandem coupling/hydrogenation catalyzed by [Cp*Ru]

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Access to 3,4- and 3,5-disubstituted piperidine derivatives has been achieved through [Cp*Ru]-catalyzed intermolecular coupling of allylic alcohols and propargylic amides. Tandem transformation was also possible *via* chemoselective [Cp*Ru]-catalyzed hydrogenation of the resulting homodienes.

In regard to their applications in pharmaceuticals, functionalized piperidine derivatives represent an important class of alkaloids and new methodologies for the preparation of substituted piperidine derivatives have attracted the attention of many researchers (Bähn et al., 2011).

Among the polysubstituted piperidines, 4-phenylpiperidine derivatives such as paroxetine, femoxetine, picenadol, pethidine, terikalant, haloperidol and related structures have found broad applications as they possess antidepressant, antipsychotic and other related biological properties (Wagstaff et al., 2002). However, straightforward access to 4-phenylpiperidine derivatives through transition metal catalysis remains scarce (Gigant et al., 2013; Despiau et al., 2014).

Recently, we reported that [Cp*Ru]-based catalysts can be judiciously employed in regioselective oxidative coupling between propargylic amines and aliphatic allylic alcohols to offer straightforward access to dehydropiperidine derivatives.20 Taking advantage of this methodology by substrate scope broadening, we now disclose that {[Ru(Cp*)(CH3CN)3]PF6} catalyzed the chemoselective semi-hydrogenation of the resulting homodienes allowing the development of tandem transformation.

In conclusion, we demonstrated that the selective oxidative coupling of allylic alcohols and propargylic amines can be extended to cinnamyl alcohol derivatives and 2-substituted allylic alcohols. This methodology allows access to 3,4- and 3,5-disubstituted enamides as valuable scaffolds for the prep aration of 3-methylpiperidine derivatives through selective [Ru(Cp*)]-catalyzed alkene hydrogenation.

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Single-click AutoDock4-based virtual screening via SwiftDock

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Abstract

Molecular Docking (MD) is an *in silico* technique employed to predict protein-ligand interactions. It can be performed using software tools such as AutoDock4 (AD4), AutoDock Vina (ADV), FlexX, GOLD, and MVD. MD is well-known for its application in virtual screening (VS), which involves docking small molecules to a macromolecule to identify lead compounds with the desired biological activity. VS can be executed using various software, including PyRx, InstaDock, and MultiDock Screening Tool, which predominantly employ ADV. Among these tools, InstaDock stands out for its single-click execution. Although several software and scripts can automate various stages of VS via AD4, no current tool is known to perform an entire AD4-based VS with a single-click execution, managing the entire workflow from protein and ligand preparation to optimal pose extraction. Therefore, we present SwiftDock (https://github.com/notacoder-dz/SwiftDock), a new open-source VS tool for Windows users capable of performing AD4-based VS in a single-click manner, requiring no prior software knowledge (MGLTools, OpenBabel, and AD4). As a demonstration, the software was placed in a folder containing protein and ligand files. Upon execution, a series of operations were carried out automatically, ranging from file preparation to post-docking extraction of the lowest binding energies and corresponding poses, employing the required software. Despite its limitations, SwiftDock aims to enhance accessibility to MD and VS for non-bioinformaticians, thereby facilitating the orientation of experimental and therapeutic research, with potential for future enhancements.

Keywords: Molecular docking; AutoDock4; Virtual screening; Single-click execution; SwiftDock

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Salt effect on the liquid-liquid equilibrium of the water/propanol/butanol-1 system

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Propanol is an alcohol widely used in many industrial applications. It is used as a solvent and cleaning agent in the pharmaceutical industry, mainly for resins and cellulose esters, as well as in the production of animal feed additives and synthetic spices.

Recovery of this alcohol from aqueous solutions is very important. Solvent extraction processes have been widely used on a production scale for liquid-liquid separation.

The choice of solvent extraction as a separation technique depends largely on the way in which the solute is distributed between the extract and raffinate phases. There are several ways of modifying this distribution in the desired way, but one of the most commonly used methods is the salt effect. Liquid-Liquid Equilibrium is the result of intermolecular forces which can significantly change due to salt addition which introduces ionic forces, affecting the thermodynamic equilibrium. In fact the presence of the salt can influence the solubility of a compound by either increasing it or decreasing it, leading to salting in and salting out, respectively.

In this study the salt effect on the system 'Water/Propanol/Butanol-1' has been studied with various salts at ambient temperature and atmospheric pressure. The salts used in the above system are KCl, $CaCl_2$ with mass fractions 5%, 10% and 15%. The solubility data and tie-line data are taken experimentally at different mass fractions of salt. It is noted that the equilibrium between phases is modified in favour of the extracted phase and the "Salting-out" effect appeared in the order $CaCl_2$>KCl. The Eisen−Joffe equation confirmed the consistency of experimental tie-line data.

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Model study of ultrafiltration membrane processes

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Abstract

Ultrafiltration (UF) is a suitable technique in a wide variety of applications, used in industrial processes such as water treatment, food industry, desalination, petroleum processing. When the particles of solute that is in the accumulated charge on the membrane surface, a low permeate velocity will be correlated with time and in parallel an increase in the concentration along the porous wall. As a result, a concentration polarization (CP) layer is developed which adversely effects on the performance of the membrane [1, 2].Therefore, numerical modeling is essential for predicting mass transfer phenomena along the membrane surface.

A tubular ultrafiltration model has been developed that couples concentration polarisation and membrane fouling. The model is based on the general convection-diffusion equation in addition to the usual membrane hydraulic resistance. The fouling due to concentration polarisation phenomenon during ultrafiltration of a solid particle of bentonite was studied. The governing equations were solved using the finite element method to simulate both wall concentration and permeate flux. The simulations were carried out at different transmembrane pressures (0.8, 1.5 and 2.5 bar), feed concentration of 1 mol/m3 and axial velocity at the inlet section of 0.59 m/s. The simulation results show that the concentration of solid bentonite particles on the membrane surface increases rapidly with time and becomes constant after a certain time. It also decreases as the transmembrane pressure increases. On the other hand, the permeate flux decreases with time up to the steady state and the increase in TMP causes an increase in the permeate flux.

Keywords: Ultrafiltration, Membrane, Numerical simulation, Fouling.

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Theoretical Study of Advanced Glycation End Products (AGEs) Inhibition: DFT Exploration of Organometallic Copper Complexes and Reactivity Descriptors.

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Abstract :

In the present work, we have theoretically examined our previously studied copper-based organometallic complexes as inhibitors against advanced glycation end products (AGEs) using Density Functional Theory DFT at wB97XD density functional with two different basis sets; DGDZVP2 and Lanl2dz. We use systematic computational analysis to investigate the key reactivity descriptors involved in the interaction of these complexes with AGEs, thereby unveiling underlying molecular mechanisms. Through untangling intricate electronic and structural characteristics, we endeavor to unveil the prime design recipes for augmenting the anti-AGE formation responsiveness of copper-organometallic complexes. Such research is crucial because it opens up new frontiers in terms of our molecular-level understanding, and provides cautionary information for designing targeted therapies to combat increasingly common AGE-related diseases.

Keywords: Density Functional Theory (DFT), Advanced Glycation End Products (AGEs), organometallic copper complexes, and the reactivity descriptors.

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Second and Third Optical Nonlinearities of Azoic Compounds and Hybrid Nanostructures.

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Abstract

Nonlinear optics (NLO), the study of the interaction of intense coherent light with matter, has significantly developed over the past few decades, profoundly influencing various technological domains. The applications of NLO materials are vast and varied, spanning optical information processing, sensor protection, and data storage. These materials are essential for advancing photonic technologies, including telecommunications and integrated optics, which are critical for the evolution of high-speed internet and other communication technologies [1].

Among the various classes of organic NLO materials, azo compound derivatives are particularly notable for their robust photochemical properties and structural versatility, which enable significant potential in photonics applications. Several derivatives of azo compounds possess a donor−π−acceptor (D−π−A) configuration, rendering them intramolecular charge-transfer (CT) chromophores. Electron-withdrawing and electron-donating substituents significantly influence the electronic spectra of azo dyes by affecting the reorganization of electronic density after photoexcitation [2].

Nanoparticles are relevant in several scientific disciplines because of their distinctive features, which markedly contrast with their bulk equivalents. These characteristics encompass an elevated surface area to volume ratio, quantum phenomena, and augmented responsiveness. Nanoparticles are used in several applications, including medical, electronics, energy, and environmental technologies [3].

This study focuses on synthesizing and characterizing highly conjugated azo compound derivatives. We discuss the synthesis protocols, characterization of the molecular structures, and third-order and Second NLO properties in the presence of nanoparticles.

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Quantification of Mineral Dust in PM10: Comparative study between two measurement campaigns (2015-2016) and (2017-2018) in Constantine

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Atmospheric particles (PM) encompass a wide range of particle types with different compositions, sizes, shapes, and optical properties [1]. They have garnered significant interest from both the public and scientists due to the substantial risk they pose to environmental [2] and human health, as they are inhalable. The WHO considers air pollution a global health priority and estimates that 1.4% of all deaths worldwide result from exposure to PM [3]. Projections indicate that air pollution's contribution to mortality could double by 2050, highlighting the challenges in managing this environmental issue [4]. Inhalation of PM10 with fine particles such as PM2.5 being one of the most invasive pollutants with undeniable health effects can trigger or exacerbate asthma, bronchitis, emphysema, and silicosis. These particles can also carry spores, bacteria, viruses, allergens, and various pollutants. Dust frequently causes eye infections, skin irritations [5], and chronic exposure to fine particles found in dust leads to respiratory and cardiovascular diseases, lung cancer, premature deaths, reduced life expectancy, and acute lower respiratory tract infections [6] [7] [8]. For these reasons, research on mineral dust has intensified in recent decades [9] [10].

Measurements mineral dust (MD) inputs are very scarce approximately the Saharan desert (SD). This work aims to identify Saharan dust intrusions, evaluate their contribution to annual and daily PM10 at an urban, and sub urban background sites located in the city of Constantine in Algeria. A reliable identification of SD days was carried out using aerosol maps provided by BSC-DREAM model and the information provided by HYSPLIT air mass back trajectories. SD is mainly composed of mineral dust (MD) due to the proximity of the Sahara to the study site. MD was determined by chemical speciation analysis and was estimated on SD days and non-SD days. The contribution of MD on SD days was about 50% higher than that observed on non-SD days. The observed average PM10 concentration during the first study period (2015-2016) was 56 ± 32.0 µg/m^3 compared to 71.26±54 µg/m^3 for the second study

period (2017-2018). The annual WHO air quality guideline (AQG) was still exceeded. Our results point out that the concentration of MD was 11.89 µg/m^3 with a contribution of 22% to the PM10 for the 1st study, and 15.84 µg/m^3 with contribution of 22% to PM10 in the second study.

These results are similar; the contribution of mineral dust in the city of Constantine is about 22% to PM10. That result confirm that the main source of particulate air pollution in Constantine is from Saharan dust.

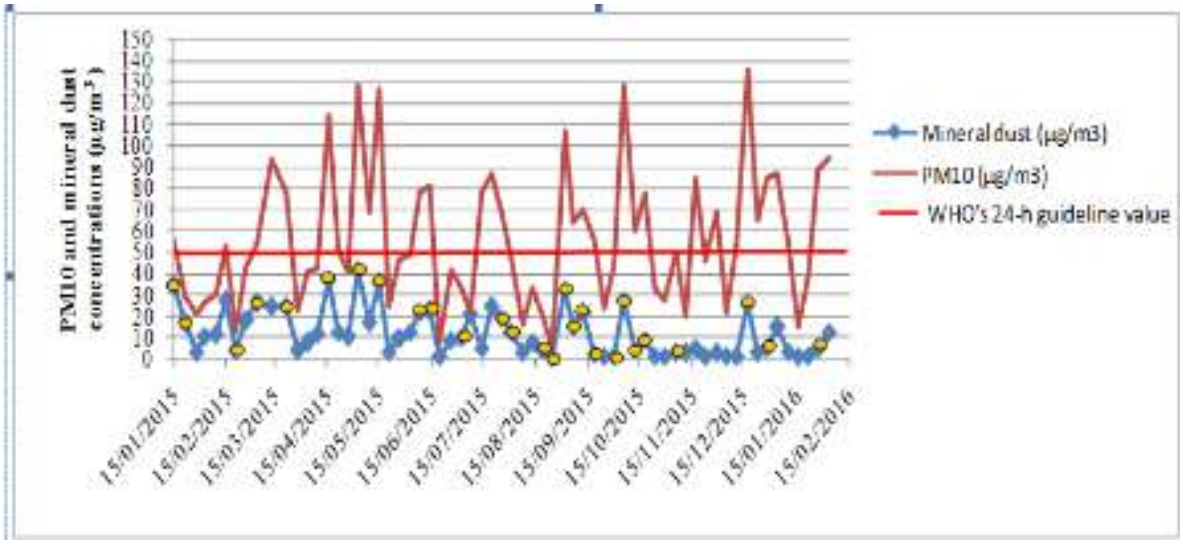


Figure 1: Annual variability of PM10 and mineral dust with WHO 24h guideline value for 2015-2016

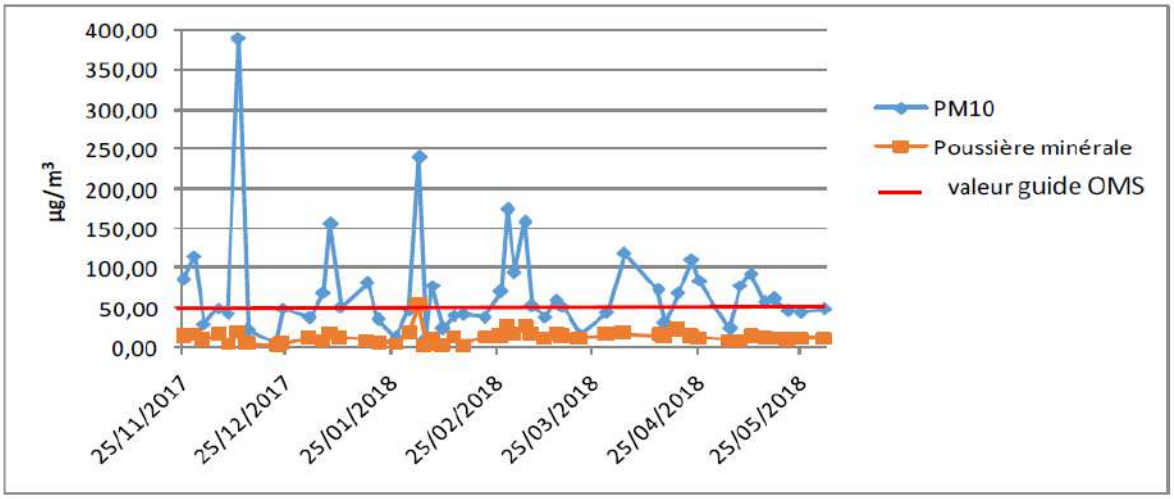


Figure 2: Annual variability of PM10 and mineral dust with WHO 24h guideline value for 2015-2016

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HPLC ANALYSIS OF A PLANT BELONGING TO THE GENUS *CONVOLVULUS*

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The natural diversity of medicinal plants has occupied researchers in extracting and separating new compounds that have a medicinal or toxic effect, compounds with biological activities, and the most important of these families is the Convolvulaceae family, which includes many genera, including the Convolvulus genus, which has many secondary metabolisms and many biological activities, the most important of which are these secondary metabolisms as follows:: alkaloids, coumarins , flavonoids, tannins, saponins, sterols and stilbenes derivatives.

hydroalcoholic extract of the aerial parts of the species Convolvulus cantabrica were evaluated using analytical HPLC technique. This analysis revealed the presence of seven polyphenols compounds.

In addition, the phytochemical study of the ethyl acetate extract of C. cantabrica, resulted in the isolation of three secondary metabolites of a polyphenolic nature. The identification of these compounds was carried out through the analysis of mass spectra ESI-MS, UV, 1D NMR (1H and 13C J-modulated and 2D (COSY H-H, HSQC J-modulated and HMBC), the measurement of rotating power and comparison with literature data.

Keyword: Convolvulaceae, Convolvulus cantabrica, secondary metabolites, polyphenol, HPLC, NMR

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BIOACTIVE COMPOUNDS AND ANTIOXIDANT ACTIVITY OF ALGERIAN PLANT

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Abstract

Phytochemicals or bioactive compounds are chemicals that present naturally in plants and they are found from various parts such as leaves, flowers, seeds and roots. From ancient times, those biomolecules including flavonoids, alkaloids, glycosides, tannins, volatile oils and terpanoids, provide defenses for plants against diseases and other environmental factors, also they are known by their uses and power treatments for humans against different ailments such as Asthma, Alzheimer and Cancers (1).

In the present study we are interested in the phytochemical study of a medicinal species which belongs to the Lithospermeae tribe and the Boraginaceae family (2). This species is a small, branched, stiff and thorny shrub with blue-purple flowers, distributed in the Saharo-sindienn from North Africa to Iran (3). The present work represents the phytochemical screening of the petroleum ether (PE) extract from this medicinal species were the results show the presence of diverse biomolecules including sterols, terpanoids, alkaloids. Moreover, two known secondary metabolites namely β-sitosterol and Daucosterol where isolated by used various chromatographic techniques including column at first step, then the precipitation in organic solvents then keep follow their purity with the Thin layer chromatography (TLC).

The antioxidant activity was evaluated on DPPH Free Radical Scavenging (2,2-diphenyl-1-picrylhydrazyl) employing different concentrations of petroleum ether extract, the results are represented in IC50 and the essays were conducted using a spectrophotometer.

Keywords: Phytochemical Screening, Bioactive Compounds, TLC Chromatography, B-Sitosterol. Antioxidant Activity.

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caractérisation physique et électrochimique du $BiVO_4$ préparé par une méthode sol-gel modifiée pour une photodégradation hautement efficace du bleu de méthylène sous irradiation solaire

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Ce travail porte sur l'utilisation du $BiVO_4$ monoclinique de type n comme photocatalyseur pour la dégradation du bleu de méthylène (MB), un colorant potentiellement dangereux. Le $BiVO_4$ monoclinique a été synthétisé par une technique sol-gel modifiée, puis caractérisé par des analyses physico-chimiques et électrochimiques. La diffraction des rayons X et MEB-EDAX a révélé la formation d'une phase unique tétragonale avec une morphologie homogène. La spectroscopie de photoélectrons X (XPS) a permis une meilleure compréhension de la composition chimique et de la structure de surface de $BiVO_4$. La réflectance diffuse (DRS) a donné une bande interdite de 2,53 eV. L'analyse BET a montré une surface spécifique de 42 m^2/g. Les courbes de Mott-Schottky ont révélé que le $BiVO_4$ présente un comportement de type n avec un potentiel de bande plate de +0,64 V/SCE (Volt vs électrode au calomel saturée) et une densité de donneurs d'électrons (Nd) de $1,46 \times 10^{16}$ cm^{-3}. Sous irradiation solaire, le $BiVO_4$ a montré une grande efficacité photocatalytique, avec une dégradation de 96 % du bleu de méthylène en 120 minutes. La cinétique de la photodégradation suit un modèle du premier ordreavec une constance de vitesse de 0,022 (min^{-1}), confirmant le potentiel du $BiVO_4$ en tant que matériau photocatalytique pour le traitement de contaminants organiques.

Mots-clés : Traitement de l'eau, Semi-conducteur, Mott-Schottky, photo-électrochimiques.

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Enhanced Photocatalytic Degradation of Paracetamol Using Silver-Doped BiOI and Bi_5O_7I Nanomaterials

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A 3D hierarchical bismuth oxyiodide (BiOI) photocatalytic material was synthesized using a simple solvothermal method. Its photocatalytic activity was evaluated by the photodegradation of paracetamol (PCT) in an aqueous solution under simulated sunlight irradiation, achieving 96% removal of PCT within 360 minutes. The photocatalytic performance of BiOI was further enhanced by doping with varying amounts of silver (Ag), ranging from 1 to 12 mol%. The results demonstrated that silver doping significantly improved the photocatalytic activity of BiOI, with performance varying according to the silver concentration. The optimal performance was observed at 9 mol% Ag-BiOI, which achieved complete removal of PCT within 120 minutes under simulated sunlight. After thermal treatment at 500°C, Ag-BiOI transformed into Ag-Bi_5O_7I, exhibiting superior photocatalytic activity compared to Ag-BiOI. The best results were obtained with 1 mol% Ag-doped Bi_5O_7I, achieving 100% removal of PCT within just 15 minutes. The significant enhancement in BiOI photoactivity can be attributed to the presence of Ag deposits acting as electron traps and the effects of high-temperature calcination on BiOI [1-3].

Keywords: Solvothermal, Ag-doped Bi_5O_7I, paracetamol, photocatalysis, water treatment

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Theoretical and Experimental Investigation of a Fluorescent Conjugated Compound

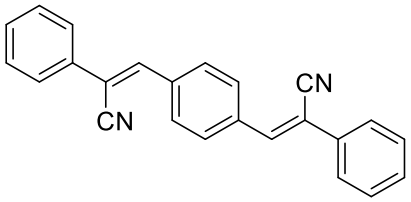
A. Marir [1], M. Guergouri[1] & R. Bensegueni[1,2]

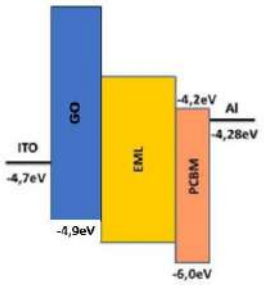
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π-conjugated organic compounds are fascinating due to their unique electronic properties, which arise from the delocalization of π electrons across a system of conjugated double bonds. This delocalization allows π electrons to move freely along the conjugated system, enabling electrical conductivity and making these compounds useful for electronics.

In this context, we synthesized 1,4-phenylene-bis(2-phenylacrylonitrile), a compound with potential applications in organic electronics. This compound was obtained via Knoevenagel condensation between terephthalaldehyde and benzyl cyanide.





Physicochemical properties were investigated using cyclic voltammetry and UV-visible spectroscopy. Optical analysis revealed that the compound absorbs in both the ultraviolet and visible regions. The visible light absorption indicates a relatively small bandgap, allowing the excitation of electrons from the valence band to the conduction band. The HOMO and LUMO energy levels were determined experimentally and theoretically. The optical, electrochemical, and theoretical bandgaps were calculated, confirming the semiconductor nature of the compound.

Its energy levels align well with TiO_2 and Al as electrodes, and graphene oxide and PCBM as charge transport layers in an OLED[1,2]. This suggests our compound is a promising candidate for the emissive layer in a bilayer OLED.

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The Effects Of Biochar On Soil Nitrogen In Arid Region

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The sustainable development of agriculture depends heavily on the soil environment. With the increase in population and food demand, the problem of diffuse agricultural pollution has become increasingly serious.

With the increase in population and food demand, the problem of diffuse agricultural pollution has become increasingly serious. Many farmers around the world have increased crop growth, using large quantities of nitrogen, causing diffuse pollution in some areas and leading to undeniable degradation of the soil environment. Biochar is used as an amendment to repair soils. According to reports in the relevant literature, biochar has a high adsorption capacity and, depending on its nature, can improve nitrogen availability in crops and fix nitrogen and other nutrients in the soil. A field experiment was carried out at the experimental station of the Department of Agronomic Sciences in Biskra to study the effect of Biochar on soil nitrogen using the Kjeldahl method. The experimental set-up included four replicates and two treatments (control and Biochar). Sampling was carried out twice after Biochar had been applied to the soil (after 3 and 8 months), at a depth of 20 cm. The results indicate that nitrogen concentrations in the second collection (after 8 months) are higher than those in the first (after 3 months), with the exception of the control and mineral fertiliser treatments. This difference in results can be explained by the variability in the rate of decomposition of organic matter and the nature of Biochar.

Key words: Nitrogen, Biochar, Mineralization, Organic amendment.

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Indicate the topic of the presentation:

- ✓ **Mathematics**

Numerical ODEs and Numerical PDEs (inc. BVPs)	Probability and Statistics
Applied Algebra and Geometry	Dynamical Systems and Algorithms

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Quantitative Structure-Activity Relationship Analysis of Imidazo[2,1-b][1,3,4]Thiadiazole Compounds Using Quantum Chemistry Approaches

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Abstract

Quantum chemistry approaches are essential for determining molecule geometries and forecasting various attributes. [1].

Quantitative Structure-Activity Relationships (QSAR) seek to establish a correlation between molecular structure or attributes derived from it and specific chemical or biological activities. [2].

All calculations were conducted utilizing HyperChem 8.03 software. [3].

A QSAR analysis was conducted on 35 imidazo[2,1-b][1,3,4]thiadiazole compounds.Multiple linear regression (MLR) is employed to quantify the relationships between molecular descriptors and the chemo-preventive properties of imidazo[2,1-b][1,3,4]thiadiazole derivatives.

The descriptors were computed using the DFT method with the STO-3G basis set. The model's predictive capability was validated using the Leave-One-Out Cross-Validation approach.

A robust correlation was noted between the experimental and anticipated values for Antiproliferative efficacy against cancer cell lines.

Keywords: imidazo[2,1-b][1, 3, 4] Thiadiazoles, Density Functional Theory (DFT), Quantitative Structure-Activity Relationship (QSAR), Multiple Linear Regression (MLR)

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Etude thermodynamique et cinétique de l'adsorption de colorant sur une biomasse

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Abstract

Au cours des dernières décennies, l'adsorption a fait l'objet de la plus grande attention en raison de son faible coût et de son efficacité dans l'élimination des polluants [1]. L'adsorption fait référence à l'accumulation de substances sur des surfaces et est utilisée pour éliminer les polluants organiques solubles. Cette méthode présente de nombreux avantages, tels que la régénération à faible coût, l'absence de boues et la facilité de récupération du matériau absorbant [2].

L'industrie textile mondiale est l'une des industries les plus dominantes parmi toutes celles qui existent. Bien que les industries textiles aient enrichi nos vies en nous fournissant des produits de valeur, elles ont également entraîné une pollution de l'environnement. Les déchets textiles contiennent des solvants halogénés hautement cancérigènes tels que le chloroforme, le dichlorométhane et le tétrachlorure de carbone. Les déchets textiles contiennent également des composés chimiques toxiques tels que des hydrocarbures aliphatiques et aromatiques, des composés contenant de l'oxygène, des sels, des métaux lourds, des enzymes, des agents oxydants et réducteurs [1, 3]. Des rapports scientifiques indiquent que les colorants peuvent perturber la photosynthèse des plantes [4], diminuer le niveau d'oxygène dissous dans l'eau et affecter la croissance générale des plantes. Par conséquent, les eaux usées textiles doivent être traitées correctement avant d'être rejetées dans l'environnement.

Diverses technologies ont été explorées pour traiter les eaux usées textiles, mais l'adsorption est le moyen le plus efficace et le plus économique de traiter les eaux usées textiles.

L'objectif de ce travail est l'étude de l'adsorption d'un colorant basique en solution aqueuse sur une biomasse afin de mettre en évidence leur potentiel comme adsorbant à faible coût pour le traitement des eaux colorées. Une étude systématique de divers paramètres tel que : quantité du support, temps de contact, concentration initiale, température, pH, a été réalisée. La cinétique, la thermodynamique et les isothermes d'adsorption ont été utilisés pour identifier les mécanismes de la rétention. Les résultats obtenus montrent que l'isotherme de Langmuir s'est avéré le mieux adapté aux données expérimentales, la capacité de sorption monocouche augmente avec l'augmentation de la température. Il a été déduit que la sorption suit un modèle cinétique de pseudo-second ordre. La nature spontanée et endothermique de la

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Synthesis and Structural characterization of tin Gadolinium Pyrochlore Gd2-xSrxSn2O7-□ (0 ≤ x ≤ 0.5) solid-oxide fuel cells (SOFC)

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Abstract

Pyrochlores oxides are oxides of general formula $A_2B_2O_7$, represent an important structure with magnetic and geometric frustrations due to the classification of cations A and B in the structure

They are named after mineral pyrochlore . They present a wide range of chemical composition variation, the ideal structural formula of the species "pyrochlore" can be written (Ca, Na) $_2Nb_2$ (OH, F) and the more general one of the group of minerals of the group $A_2B_2O_7$ The site A may be occupied by Na, Ca, Sr, Mn, La, etc.; site B can be occupied by Nb, Ta, Ti, Sn and O. [The ideal $A_2B_2O_7$ pyrochlore structure is commonly described as a derivative of the fluorite structure where the scheduling of type A and B cations at two sites results in a doubling of the unit cell to about 10.5 Å.

The oxide can be written $A_2B_2O_6O'$ with cubic coordination space group Fd-3m.
The work described in this paper is devoted to the synthesis and characterization of a pyrochlore structure based on Gadolinium (Gd_2O_3) and tin (SnO_2) oxides of general formula $Gd_2Sn_2O_7$, substituted by Sr at the site Gd . Their structures were determined from X-ray powder diffraction using Rietveld analysis. All the compositions present the space group Fd-3m.

Keywords X-ray, pyrochlore, Rietveld analysis, synthesis

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Traitement de l'eau polluée par le méthyle orange: application des procédés d'oxydations avancées sur CeO_2

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Ce travail a pour objectif l'étude de l'adsorption du méthyle orange comme colorant anionique dans le milieu libre et sa dégradation catalytique par les procédés d'oxydation avancées en utilisant CeO_2 synthétisée par la méthode de sol-gel.

Les principaux résultats de MEB-EDAX à éprouver la composition chimique de CeO_2; le pourcentage atomique d'oxygène (8.33%) et le cérium (88.4 %), Le spectre de DRX de l'échantillon confirme la présence de phase de CeO_2, le spectre FTIR-ATR confirme les bandes caractéristiques de ce dernier. Les résultats obtenus par la caractérisation de BET ont montré une importante surface spécifique (51.74 m^2/g).

Les études de cinétique et d'équilibre d'adsorption de MO ont été réalisées en conditions batch dans les conditions suivante (pH libre, R=1g/L, [MO]=50 mg/L). L'étude cinétique a révélé que la réaction de surface s'adapte au modèle de pseudo-second ordre. Le rendement d'adsorption est de 28.43%.

Les résultats et les conditions de l'étude d'élimination de MO par POAs sur CeO_2 sont comme suite :

Pour le Fenton-like et photo Fenton-like l'équilibre d'adsorption a été réalisé selon les conditions suivante: teq=60 min, [MO] = 50mg/L, pH = 6. Après l'ajout de [H_2O_2] =150 mM, nous observons une dégradation moyenne de 45.54% avec le procédé Fenton-like ; et 60.72 % avec le procédé photo Fenton-like pendant 2 heures [1], [2], [3].

Mots-clés : Traitement de l'eau, Méthyle Orange, adsorption, POAs, CeO_2.

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Coordination polymer of Alkaline-Earth Based on polucaeboxylic acid, Synthesis, Structure and Characterization.

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Abstact:

Single crystals of strontium coordination polymer, [Sr(H_4BTEC)(H_2O)] (I), (H_4BTEC=1,2,4,5-benzenetetracarboxylicacid), was synthesized hydrothermally and characterized by single-crystal X-ray diffraction, powder X-ray diffraction, scanning electron microscopy (SEM-EDX), thermal analysis (TG-MS) and DSC. The single-crystal structure analysis showed that compound (1) displays a 2D structure and crystallizes in the monoclinic space group C2/c, and the center atoms coordinate to seven oxygen atoms from five different H_4BTEC^{2-} anions and one oxygen atom belonging to one coordinated water molecule with eight-coordinated distorted bicapped prism. The luminescent property of the title complex has been investigated.

Key words: Coordination polymers, hydrothermal synthesis, X-ray diffraction.

1. Introduction

Coordination polymers (CPs) consisting of inorganic metal ions or clusters and organic ligands, which may generate a huge number of novel interpenetration networks ,have become one of the fast et growing fields in chemistry and at tract immese interest**[1–5]**.

2. Results and discussion

The compound crystallizes in the monoclinic space group *C2/c*. Details of the data collection and structure refinement, atomic coordinates and occupancy. The asymmetric units of compound (I) comprises, one Sr^{2+}, one partielly deprotonated H_4BTEC^{2-} anions and one water molecule O1W. The coordination arrangement of the Sr atom is eight-coordinated

distorted bicapped prism. Its coordination sites are accupied by seven oxygen (O1, O1^{iv}, O2, O2^{iv}, O5^{iii}, O6^{iii}, O7^{ii}) from five different H_4BTEC^{2-} anions and one oxygen atom belonging to one coordinated water molecule O1W (Fig.1). The Sr–O (carboxylate) bond lengths range between 2.491(2)-2.824(2) Å. The Sr–O(aqua) bond lenght is 2.525(3) Å. These distances are comparable to those reported in other strontium-carboxylate complexes **[6]**.

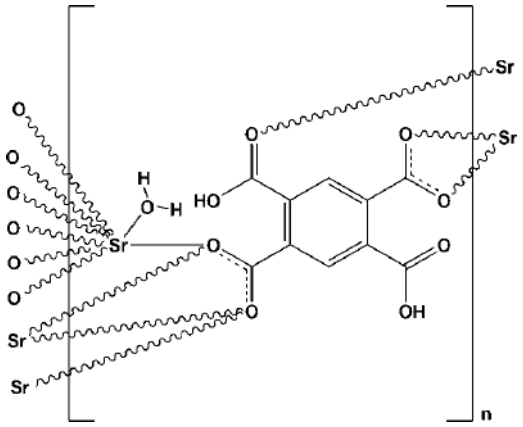


Fig.1: Different coordination preferences of the metal ions.

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Synthesis of a new material based on phenylene cyano vinylene and its application in organic electronics

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Organic π-conjugated oligomers and polymers constitute an important class of functional materials in organic electronics. They are used as active layers in organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs) or in organic solar-cells (OSC). In this latter application, efficient materials usable as p-conducting layer in bulk-heterojunction (BHJ) solar cells in association with fullerene derivatives as n-conducting materials are needed [1, 2] In fact, a material with a bandgap of 1.1 eV is able to absorb 77 % of the solar irradiation, however, semiconducting polymers or oligomers have bandgaps higher than 2 eV and can then harvest only 30 % of the solar photons.

In the last few years, the scientists seek to synthesize organic molecules having gaps similar to those of metals. Recent studies showed that the family of the poly (thienylenevinylene) (PTV) presents a gap electronic Eg lower than that of polythiophen (Pt), 1.8 and 2.1eV respectively. Other work showed that the introduction of an acceptor group into the combined chain has an advantage in the control of this forbidden band. Indeed, the substitution of the electron-withdrawing cyano group in the double connection of the poly (thienylenevinylene) leads to a polymer with a great electronic affinity.

We have synthesized monomers to study a class of soluble low band gap conjugated polymers based on heterocyclic units and cyano vinylenes. We report a sample study of one of this class of material, the poly (2Z, 2'Z)-2, 2'-(1, 4-phenylene) bis (3-(furan-2-yl) acrylonitrile).

The poly (2Z, 2'Z)-2, 2'-(1, 4-phenylene) bis (3-(furan-2-yl) acrylonitrile) film was synthesized electrochemically by anodic way in an electrolytic bath of Bu_4NPF_6 (0,2M)/CH_2Cl_2 with anhydrous conditions and under inert atmosphere. The polymer formed on Pt or ITO electrode, either by cyclic voltammetry or by potentiostatic method, was characterized by spectroscopic methods, IR, UV.

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ECO-FRIENDLY APPROACH TO DIHYDROPYRIMIDINONE SYNTHESIS VIA THE BIGINELLI REACTION

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The Biginelli reaction, a multi-component condensation, affords 3,4-dihydropyrimidin-2(1H)-ones/thiones (DHPMs)[1] .This investigation delves into the influence of eco-friendly solvent alternatives, specifically deep eutectic solvents (DESs)[2], on reaction stereoselectivity, yield, and product purity. Our findings demonstrate the efficacy of DESs in enhancing Biginelli reaction yields. Comprehensive characterization through proton nuclear magnetic resonance (^{1}H NMR), high-performance liquid chromatography (HPLC), and infrared (IR) spectroscopy furnished invaluable insights into the performance of each experimental protocol.

Keywords: Biginelli reaction; Catalyst; deep eutectic solvents; Stereoselectivity; 3,4-Dihydropyrimidin- 2(1H)-ones

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Assessment of the Corrosion Inhibition Performance of Ephedra Extract on Ferrous Metal Alloys in Acidic Media: Electrochemical and Gravimetric Studies.

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Abstract:

Corrosion, a significant economic and safety concern, poses a substantial threat to various industries. Traditional synthetic corrosion inhibitors often carry environmental and health risks, motivating the search for greener alternatives. Plant-based extracts have emerged as promising candidates due to their natural composition and potential for sustainable production. This study investigated the corrosion inhibition properties of an extract derived from a species of Ephedra, a genus of flowering plants commonly found in arid regions. The extract was evaluated for its effectiveness in protecting API 5L X70 carbon steel, a widely used material in oil and gas pipelines, from corrosion in a 1M hydrochloric acid (HCl) solution. Electrochemical techniques, including Open Circuit Potential (OCP), Potentiodynamic Polarization Curves, and Electrochemical Impedance Spectroscopy (EIS), were employed to assess the extract's inhibitory performance. Additionally, weight loss measurements were conducted to quantify the extent of corrosion. The results demonstrated that the Ephedra extract exhibited exceptional corrosion inhibition capabilities. At an optimal concentration of 400 ppm, the extract achieved a maximum inhibition efficiency of 82.81%. Scanning Electron Microscopy (SEM) analysis further confirmed the protective effect of the extract on the metal surface.

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DFT Evaluation of Macrocyclic Compounds for Reducing Polycyclic Aromatic Hydrocarbon Toxicity in Pollution Control.

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Abstract

This study investigates the theoretical aspects of encapsulating Anthracene, a toxic polycyclic aromatic hydrocarbon (PAH) [1], using cucurbiturils (Q[6], Q[7], and Q[8]) [2]. This research aims to contribute to pollution control technologies and environmental health strategies through a deeper understanding of molecular interactions.

Utilizing quantum mechanical methods, including PM7 and density functional theory (DFT) with dispersion corrections [3, 4], we evaluated the stability and complexation energy of Anthracene with these cucurbiturils. Among the complexes studied, Anthracene@Q[7] demonstrated the most stable configuration, exhibiting a complexation energy of -53.81 kcal/mol, followed by Anthracene@Q[6] at -51.84 kcal/mol. Conversely, Anthracene @Q[8] displayed the lowest stability, indicating weaker interactions and less favorable thermodynamic properties.

The analysis highlights the critical role of non-covalent interactions, such as π–π stacking, in stabilizing these complexes[5]. Furthermore, we assessed electronic properties, including the HOMO and LUMO levels, with Anthracene@Q[7] showing the highest HOMO energy (-7.43 eV), indicating a greater propensity for electron donation compared to the other complexes. The observed variation in energy gap for Anthracene@Q[7] underscores its potential for environmental applications, particularly in the detection and remediation of toxic PAHs like Anthracene.

These findings enhance our theoretical understanding of cucurbiturils, particularly Q[7], in environmental remediation, offering valuable insights for the development of innovative pollution management technologies.

Keywords: Cucurbiturils, Pollution Control, PAH, Anthracene, Quantum Simulations.

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Chemical Pathways for Hydroxyapatite Extraction from Local Phosphate Sources

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Calcium phosphate-based ceramic biomaterials have been widely used as bone substitutes for about 20 years in different medical fields. Additive manufacturing is an ideal solution to shape and manufacture medical implants due to its ability to 3D print patient-specific personalized products. Most researchers in this field are interested in randomly distributed pores or simple architectures in scaffolds. Control of porosity, pore size and distribution is necessary to obtain implants with mechanical properties close to those of bone and to ensure their osseointegration. The aim of the present work was therefore to develop and characterize such a specific porous structure.

The first part of our work, focused on chemistry and more particularly inorganic chemistry, consists of the extraction of hydroxyapatite from local phosphate. The objective of this method is to obtain pure hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$, using local phosphate resources. This extraction involves a dissolution step with nitric acid to solubilize the phosphate, followed by a controlled precipitation of the hydroxyapatite using ammonia.

This allows the production of a valuable biomaterial used in particular in the medical field for applications such as implants and bone grafts, in addition to valorizing local resources.

Key Words: Hydroxyapatite, bone substitutes, dissolution, precipitation.

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A DFT and molecular docking study on potential 5α-reductase inhibition derived from Ficus carica L that promote hair growth.

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Androgenic alopecia (AGA) is a common condition linked to high levels of dihydrotestosterone (DHT), which is produced from testosterone by the enzyme 5α-reductase. Our research has shown that bioactive compounds from the leaves and fruit of Ficus carica L, particularly the triterpenoids constituents, which can inhibit the activity of 5α-reductase. We used density functional theory (DFT) calculations to identify the optimal molecular structures and the conceptual DFT to determine the active sites. Besides, the molecular docking study was used to analyze how these compounds block 5α-reductase and to predict their biological effects. We calculated several chemical properties, such as energy levels and reactivity, to understand how these compounds might interact with the 5α-reductase enzyme. The docking results indicate that these compounds can effectively bind to the 5α-reductase receptor, suggesting that Ficus carica L. could be a promising natural treatment for AGA.

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Photocatalytic properties of bio-synthesized Zinc oxide nanoparticles from eucalyptus plant

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Heterogeneous photocatalysis with zinc oxide nanoparticles has been demonstrated as an emerging semiconductor material and widely been used in the treatment of wastewater due to its inertness, strong oxidizing power, and nontoxicity [1].Therefore, various chemical, physical, biological, and green synthesis approaches have been developed to synthesize ZnO NPs [2]. The most abundantly used biological route for NPs synthesis is the use of plant extracts for the formulation of ecofriendly NPs, which cuts out the use of noxious chemicals with toxic effects [3].

The main aim of this study is to synthesize green zinc oxide NPs, using the reducing zinc nitrate in the fresh aqueous leaf extract of the plant Eucalyptus, and evaluation of photocatalytic activity under UV-Visible irradiation for degradation of methylene bleu as model of toxic dye. Zinc oxide NPs synthesized by leaf extract results were compared to commercial ZnO, and the combined methods of synthesis were investigated and reported.
Photochemical oxidation experiments were carried out under UV (365nm) and solar irradiation in order to evaluate and compare the performance of the processes.

The results revealed that green synthesized zinc oxide NPs exhibited efficient photocatalytic activity under sunlight compared to UV irradiation, and this is confirmed by the rapid disappearance of dye especially under sunlight than artificial irradiation. The results of comparative study showed that the k_{app} for the both photocatalysts (biosynthesized and commercial ZnO) is almost identical, which confirms the significant performance of the biosynthesized material. This is due to the alterations in band gap, structural changes and surface area in nanoparticles that increased the activity. Also, the functional groups of biosynthesized materials were confirmed by FT-IR spectroscopy and XRD.
The biosynthesis of the photocatalyst nanoparticles presents promising performances in the field of water treatment which require additional studies.

Keywords: green synthesis, *Eucalyptus*, solar irradiation, ZnO, photocatalytic activity.

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A comparative study on modified electrodes utilizing MWCNTs for lead trace detection: Recent studies

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Abstract: Recent studies on modified electrodes utilizing multi-walled carbon nanotubes (MWCNTs) for lead detection highlight various innovative approaches:
1-Screen-Printed Carbon Electrode: A copper film-modified MWCNT electrode achieved a low detection limit of 1.2×10^{-10} M for lead, demonstrating effectiveness in field conditions [1].
2-Carbon Paste Electrode: Another study reported a novel carbon paste electrode with MWCNTs and poly 4-N-pyridine para styrene sulfonamide, achieving a detection limit of 6.0×10^{-9} M and a linear range from 1.0×10^{-1} to 1.0×10^{-8} M [2].
3-Potentiometric Sensors: MWCNT-functional ionophore-based sensors were developed, showing selective lead detection in water with promising sensitivity [3].
These studies demonstrate the potential of nanocomposite carbon-based modified electrodes for trace metallic detection in water. The unique properties of carbon nanotubes, such as their high surface area and electrical conductivity, make them suitable for enhancing the performance of electrodes in trace metallic detection applications.

Keywords: Multi-walled carbon nanotubes MWCNTs, Lead trace, Modified electrodes, Electrochemical detection.

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Synthesis and optimization of the condensation reaction between flavanones and diamines: towards novel functional molecules

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This study aims to develop an efficient synthesis of imines from the condensation of flavanones and diamines. We have explored the influence of various reaction parameters on the yield and selectivity of this transformation.

Experiments were conducted under nitrogen atmosphere and protected from light to prevents oxidation reactions and unwanted photochemical reactions. The influence of temperature –(room temperature, reflux, 50°C)- and reaction time –(1 day to 4 days)- on the yield and purity of the products was studied. Various solvents were tested concerning reaction conditions that can influence the solubility of reactants and the rate of reaction.

The obtained products were characterized by spectroscopy methods (NMR and IR). Temperature and reaction time strongly affect yield and selectivity-as was also revealed by our results. Optimized reaction conditions enabled us to obtain the target imines in very high yields.

These optimized reaction conditions open new perspectives in the preparation of functional molecules with interesting properties, mainly in the areas of medicinal chemistry and material sciences.

Keywords: flavanone, diamine, imine, condensation, optimization, yield, selectivity, NMR, IR, TLC.

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Synthesis of Cyclodextrin-Encapsulated Iron and Catalysis for the Polymerization of Ethylene

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Although dominated by the very active Group 4 metal- locenes catalysts for a long time,[1] the field of catalytic polymerization has recently been rejuvenated by Brookh- art[2] and Gibson's seminal works[3,4] on the use of late transition metal complexes in olefin polymerization. Beside systems containing the α-diimine ligand framework,[5] ni- trogen-containing tridentate complexes of iron and cobalt based on the 2,6-bis(iminoaryl)pyridine fragment are amongst the most studied because of their ability to pro- mote the formation of linear polyethylene very efficiently.[6] Steric bulk control around the metal center is a prerequisite not only for forming the neutral trigonal-pyramidal MCl_2 catalyst precursor at the expense of the inactive octahedral cationic $[(N,N,N)_2Fe]^{2+}$complex,[7] but also for tuning the molecular weight of the polymer produced.[4] So far, the control of the steric environment at the metal has been achieved by changing the size of the aryl (Ar) and imino carbon (R) substituents of the 2,6-bis(iminoaryl)pyridine moiety. An alternative would be to encapsulate the metal fragment in molecular cavities of various sizes. Here we de- scribe the synthesis of methylated α- and β-cyclodextrin (CD) derivatives[8] rigidly capped with a 2,6-bis(imino)pyri- dyl fragment and the activity of their iron complexes in ethylene polymerization.

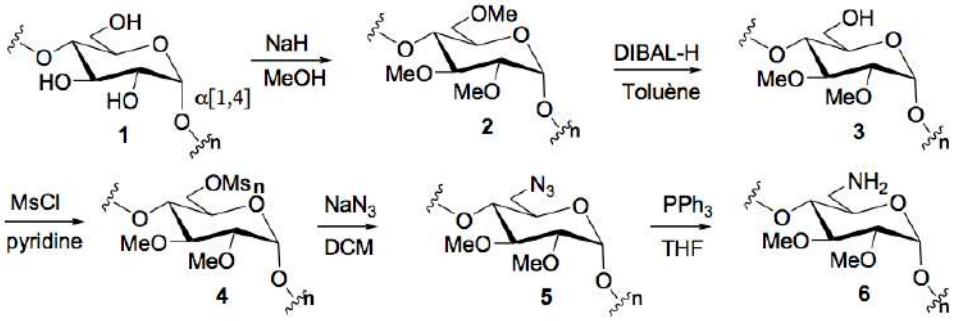


Figure 1. Synthetic general scheme.

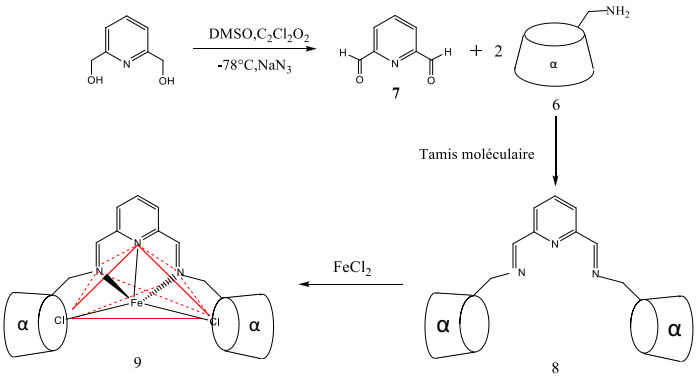


Figure 2. Condensation and complexation scheme.

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The influence of Fe, Cu, and Mn addition on the mechanical properties and corrosion behavior of novel biodegradable Zn-based alloys prepared by powder metallurgy

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Abstract:

Metals and their alloys have been important in reconstructive surgery, especially orthopedic surgery [1]. The focus on degradable metallic materials has led to research hotspots and clinical demands. In the past, bioinert metallic materials have been used in biomedical implants. However there have been some long-term complications after surgery, and usually, patients need to have another surgery, which may cause more problems [2]. Biodegradable metals have been proposed to disappear slowly in the human body during and after their service. Recently, zinc (Zn) and its alloys have been considered promising biodegradable materials due to their moderate degradation and acceptable biocompatibility. However, poor mechanical performance limits its clinical application [3]. In this work, a systematic study of different alloying elements Fe, Cu, and Mn was conducted to investigate their effects on the microstructure, mechanical properties, and corrosion resistance of Zn-1Mg alloys produced by powder metallurgy. The morphological and structural characteristics of samples were analyzed using an optical microscope, scanning electron microscopy/energy dispersive X-ray spectroscopy (SEM/EDS), and X-ray diffraction (XRD). Electrochemical and immersion tests characterized its corrosion behavior under simulated body fluid at 37 °C. The results showed that adding elements such as Cu, Fe, and Mn improved the mechanical properties of the Zn-1Mg alloy. The corrosion test in the SBF solutions shows that the corrosion rate of the ternary Zn-1Mg-0.5Cu alloy was less than two times lower than that of Zn-1Mg binary alloy (0.15 mmpy). Based on the experimental results, the Zn-1Mg-0.5Mn alloy has the best properties and is therefore a better biodegradable alloy for implant applications.

Keywords: Zinc biodegradable alloy, powder metallurgy, corrosion

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Energy decomposition analysis of aminopolycarboxylic acids: An EDA approach

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Intermolecular interactions play a crucial role in determining the physicochemical properties of molecular systems. The energies of these interactions are typically calculated using theoretical methods such as Hartree-Fock (HF), MP2, and CCSD(T). The Energy Decomposition Analysis (EDA) method was originally developed by Morokuma and later refined by Ziegler and Rauk [1]. This method involves performing DFT calculations on each fragment in isolation, allowing for the breakdown of intermolecular interactions into distinct energy components:

$$\Delta E_{int} = \Delta E_{orb} + \Delta E_{elect} + \Delta E_{pauli} \qquad (1)$$

In the context of mono-electronic approximation, orbital interaction energyΔE_{orb} represents the stabilizing interactions between two electrons and their respective orbitals.

The electrostatic energy ΔE_{elect},represents the interaction between fragments, calculated based on their electron density distribution.

Pauli repulsion energyΔE_{pauli} arises from the fact that two electrons with the same spin cannot occupy the same region in space, leading to a destabilizing effect.

This quantitative analysis seeks to evaluate the significance of ionic and covalent interactions in the coordination bonds of M-EDTA and M-EDDS complexes (M = Ni, Zn, Fe). The energy decomposition follows equation (1), based on the original method developed by Morokuma and subsequently enhanced by Ziegler and Rauk [2].

Keywords: EDA, DFT, EDTA, EDDS

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Optimization of Pyrolytic Conditions for Date Palm Seed Biochar: Advanced Characterization and Adsorption Potential for Environmental Remediation

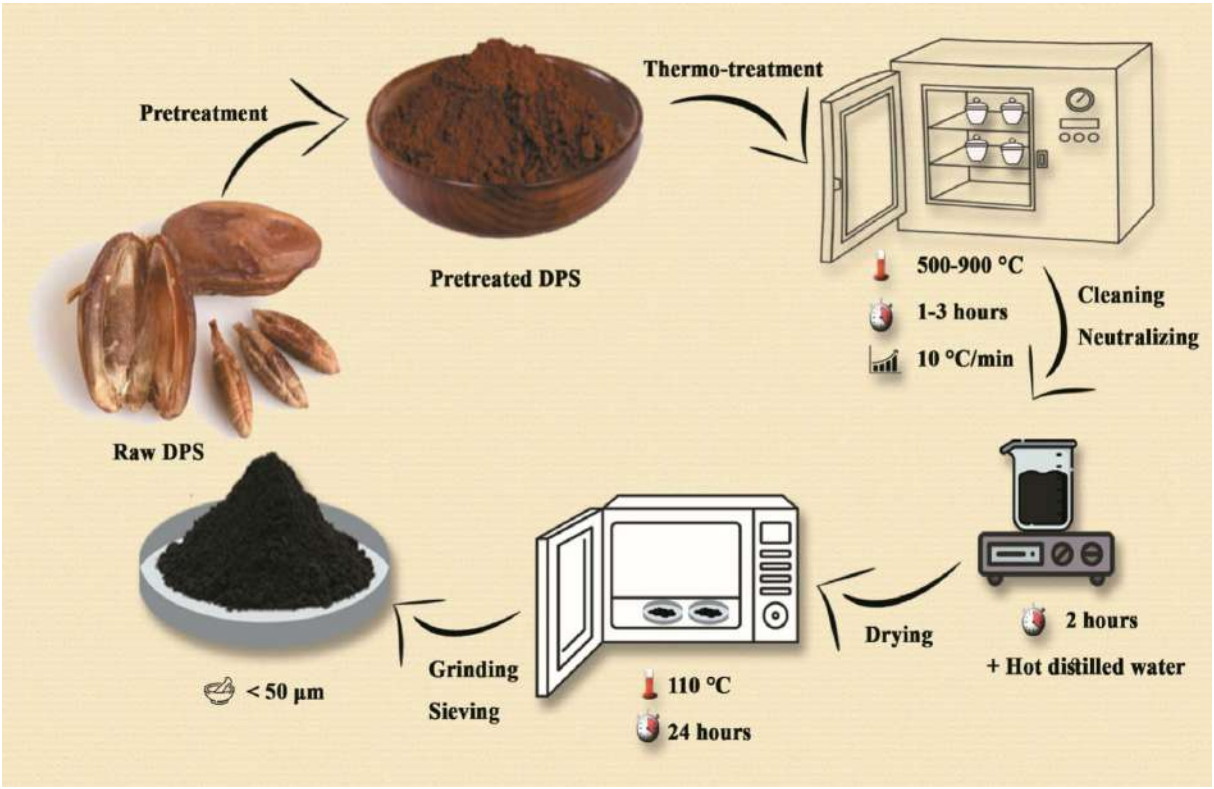
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This study focuses on the optimized pyrolytic synthesis and physicochemical characterization of biochar derived from date palm seeds (DPS), a widely available agricultural waste in arid regions. The primary objective was to enhance biochar properties for environmental remediation through the use of response surface methodology (RSM) combined with central composite design (CCD). By varying pyrolysis temperature (600–900°C) and duration (1–3 hours), the study optimized critical factors like specific surface area, micropore volume, and yield. The best-performing biochar was produced at 828°C with a pyrolysis time of 1.7 hours, resulting in a specific surface area of 654.8 m^2/g, micropore volume of 0.190 cm^3/g, and a yield of 30.5%. Comprehensive physicochemical characterization techniques, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) with energy-dispersive X-ray spectroscopy (EDS), and Brunauer-Emmett-Teller (BET) surface area analysis, were employed to understand the biochar's structural and compositional attributes. XRD revealed an amorphous carbon structure with some graphitic domains, while FTIR detected functional groups such as hydroxyls and carbonyls that are crucial for adsorption. SEM imaging showed a highly porous structure, and BET analysis confirmed a large surface area and well-developed microporosity. The biochar's point of zero charge (pHpzc) was measured at 7.58, indicating its potential for selective adsorption of both positively and negatively charged contaminants depending on the pH. The experimental data closely matched the RSM-predicted results, validating the effectiveness of the optimization process. This research demonstrates that DPS-derived biochar, with its high surface area and microporous structure, is a promising adsorbent for environmental remediation. Its production from waste materials aligns with sustainable resource management and circular economy principles. Future work should focus on scaling up the production process, evaluating real-world applications in wastewater treatment, and exploring further modifications to enhance the biochar's performance for specific environmental pollutants.

Keywords: Biochar optimization; Pyrolysis; Date palm seeds; Environmental remediation; Response surface methodology; Adsorption potential



Synthesis journey and methodological innovation in BC preparation

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Synthesis and Biological Evaluation of Ferrocene Derivative Compound: A Combined In Vitro and In Silico Study

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Inflammation is a multifaceted, dynamic reaction to cellular damage, infection, trauma, or toxins, which may persist for a brief period (acute inflammation) or an extended length (chronic inflammation). Uncontrolled inflammatory processes are the fundamental cause of several human diseases, including cancer, diabetes, arthritis, gastrointestinal, cardiovascular, and neurological problems. Derivatives of ferrocene have garnered considerable attention due to their powerful biological actions against many illnesses. This research seeks to elucidate the function of Ferrocene derivatives in the treatment of inflammatory disorders by in-silico and in-vitro analyses. The specificity and binding affinity of Ferrocenylmethyl aniline were assessed by molecular docking analysis. The present research seeks to understand and establish the function of the Ferrocene derivative in the treatment of inflammatory disorders via in-silico and in-vitro experiments. The study used the in silico docking approach, using the chemical molecule Ferrocenylmethyl aniline and a protein model of BSA obtained from the Protein Data Bank (PDB), followed by the docking procedure executed with the AutoDock Tools 1.5.7 software. The in vitro procedure included the manufacture of the Ferrocenylmethyl aniline molecule and an investigation of its interactions with bovine serum albumin (BSA). The findings indicate that these ferrocene compounds have an electrostatic interaction with BSA, and the IC50 value demonstrates markedly greater activity in comparison to Diclofenac. The overall findings indicate that the Ferrocene derivative exerts its anti-inflammatory effects via direct interaction with BSA. Ferrocenylmethyl aniline may serve as an effective compound in the management of certain inflammation-related disorders.

Keywords: Ferrocenylmethyl aniline, BSA, anti-inflammatory activity, Docking

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Eco-Friendly Adsorption Approach for Dye Removal Using Agricultural Wastes as Adsorbents

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Abstract

Industrial effluent streams frequently contain a variety of pollutants and synthetic dyes that pose significant risks to human health and aquatic ecosystems. Among these pollutants, dyes are particularly concerning due to their toxicity, non-biodegradability, and potential to cause mutagenic and carcinogenic effects. As a result, the removal of dyes from wastewater has become a pressing environmental issue. This study explores the potential of two different natural adsorbents (agricultural waste) specifically pea peel powder, and raw pine tree bark (RPTB) for the removal of crystal violet from contaminated water. Both materials offer a sustainable, low-cost alternative to conventional adsorbents, and their efficiency in dye removal is compared under similar experimental conditions.

A batch-mode adsorption process was used to investigate the effects of various physicochemical parameters on dye removal efficiency, including contact time, initial dye concentration, adsorbent dosage, pH, and temperature. The kinetic behavior of the adsorption process was analyzed using pseudo-first-order and pseudo-second-order models. In both cases, the pseudo-second-order model provided the best fit, suggesting chemisorption as the predominant mechanism for dye uptake. Adsorption isotherms were also evaluated using the Langmuir and Freundlich models. While the Freundlich isotherm model was found to accurately describe the adsorption behavior for both pea peels and pine bark, it was particularly indicative of the heterogeneous surface properties of the adsorbents.

The comparison between pea peels and raw pine bark focused on their adsorption capacities and efficiency across different concentrations and temperatures. Both adsorbents demonstrated effective dye removal, though each displayed distinct adsorption characteristics. Pea peels, as a readily available agricultural by-product, showed promise as a highly cost-effective option for areas with access to agricultural waste. On the other hand, raw pine bark, a forestry by-product, offered comparable adsorption efficiency, making it a viable option in regions where forestry waste is abundant.

The thermodynamic studies for both adsorbents revealed key insights into the nature of the adsorption process. The positive values of the standard enthalpy change (ΔH) for both

materials confirmed the endothermic nature of the adsorption, indicating that temperature played a crucial role in influencing the adsorption capacity of both materials.

In conclusion, both pea peel powder and raw pine tree bark exhibit significant potential as eco-friendly and cost-effective adsorbents for the removal of synthetic dyefrom wastewater. These natural materials, derived from agricultural and forestry waste, provide a sustainable solution to one of the most pressing environmental challenges posed by industrial dye pollution. By utilizing locally available waste products, these approaches not only help mitigate the hazards of dye contamination but also promote waste valorization in a circular economy.

Keywords: adsorption, synthetic water, agricultural waste, kinetics, isotherms, dye removal.

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Theoretical modeling using DFT and TDDFT methods of a nickel complex for photovoltaic applications.

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Extensive research is currently underway on Grätzel-type photovoltaic cells. In this type of cell, a crucial factor that determines the efficiency of an organic photovoltaic cell is the “dye sensitize'” or optical dye. The photovoltaic effect is defined as the direct conversion of electromagnetic energy (radiation) into direct electric energy. These cells are made up of semiconductors and dye sensitizers.

In the field of coordination chemistry, Schiff base compounds play a vital role, especially in the formation of Schiff base complexes. These ligands are significantly important because they have the potential to form stable metal complexes. [1] These complexes and their ligands are the focus of extensive research due to their numerous applications. "They have proven to be effective and stereospecific catalysts for reactions such as oxidation, reduction, hydrolysis, and other transformations of organic and inorganic compounds [2] as well as for use in dyes, pigments, and optoelectronic devices.[3]

Our study centers on the theoretical analysis of a specific nickel-based complex, Bis{1-[(o-tolyl)iminomethyl]-2-naphtholato}nickel(II), in both the gas phase and solvated conditions By employing computational methods such as DFT and TD-DFT, we seek to comprehensively analyse the structural, electronic, and optical properties of this complex, along with its potential for photovoltaic conversion.

Keywords: Schiff base, photovoltaic cell, DFT, TDDFT,

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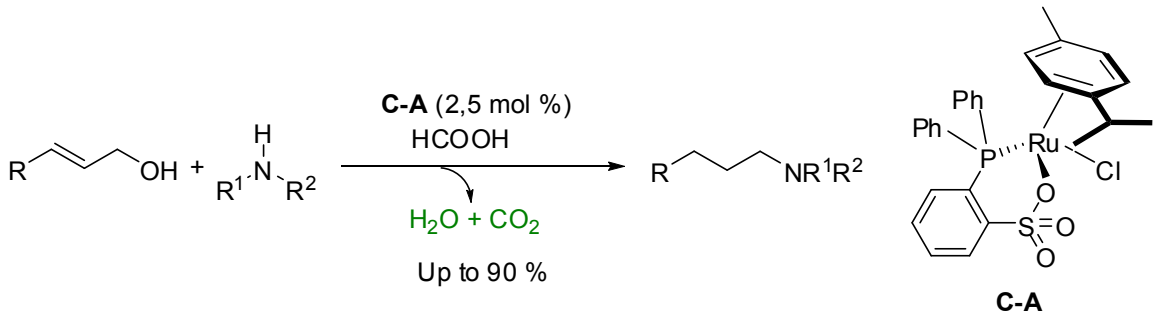
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Ruthenium-Catalyzed Reductive Amination of Allylic Alcohols

Zeyneb Sahli,[1] Basker Sundararaju,[2] Mathieu Achard[2] and Christian Bruneau[2]
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Catalytic reactions involving hydrogen (auto)transfer, generating only water and non-toxic salts as byproducts are particularly clean, efficient and attractive methods from a sustainable point of view for the valorization of terpenes. [1] In this context we have developed a new and efficient catalytic system for reductive amination of allylic alcohols in the presence of various amines using arene ruthenium(II) complex.[2]The application of this method to a wide range of terpenic allylic alcohols like geraniol, nerol and phytol allowed the formation of new azaterpenes in good yield and high chemoselectivity generating only water and carbon dioxide as benign side products.(Scheme)



Sheme. *Ruthenium(II) catalyzed reductive amination of allylic alcohol.*

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Natural bond orbital and molecular electrostatic potential analysis of polyoxotantalates

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Polyoxotantalates (POTas), a class of polyoxometalates composed of tantalum and oxygen atoms, have gained siginificant attention in recent years due to their intriguing structural diversity and versatile applications in catalysis, materials science, and medecine [1].

In order to get clear insight on how molecular structure can influence the reactivity of these compounds, theoretical study on five distinct heteropolyoxotantalates, namely Se_4Ta_6, Se_2Ta_6, P_4Ta_6-cis, P_4Ta_6-trans, As_4Ta_6 comprising the same addenda tantalum atom and different heteroatoms (Se, P, As) is carried out using Density Functional Theory (DFT) :

Natural Bond Orbital (NBO) analysis is an efficient method for interactions among bonds. It is performed to describe the charge transfer in molecular systems [2].

Molecular Electrostatic Potential (MEP) can be used to find what region of molecule is electron rich or poor to have an interpretation what side of molecule is apt for nucleophilic or electrophilic attack [3].

Keywords : Polyoxotantalates, DFT, NBO, MEP.

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Synthesis, Characterization, and Biological Evaluation of Silver(I)-*N*-Heterocyclic Carbene Complexes and their Benzimidazolium Salt Precursors: Investigating their Anti-Lipase and anti-alpha-amylase Potential

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Abstract:

This study reports the synthesis and comprehensive characterization of novel silver(I)-*N*-Heterocyclic Carbene complexes and their benzimidazolium salt precursors. The main objective of this investigation was to delve into the inherent capabilities of these synthesized compounds, particularly their potential as potent inhibitors with remarkable biological activities. Rigorous in vitro assessments were conducted to ascertain their effectiveness in terms of anti-lipase and anti-diabetic properties. Encouragingly, the results demonstrated that the silver(I)-NHC complexes (3a-f) demonstrated considerable efficacy against both enzyme types. Notably, their strongest activity was manifested against α-amylase enzymes. Although their effectiveness against the lipase enzyme was slightly lower compared to established reference drugs, a notable inhibitory effect was still observed. In stark contrast, the benzimidazolium salts 2a-f, despite their structural similarity, exhibited negligible activity against both lipase and α-amylase enzymes. These findings highlight the promising inhibitory potential of silver(I)-NHC complexes as candidates for further development in anti-lipase and anti-diabetic therapies.

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Iron-TiO_2 Pillared Clay Nanocomposites: Sustainable Approaches for Photocatalytic Elimination of Organic and Pathogenic Contaminants.

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The synthesis of modified natural bentonite using TiO_2 nanoparticles, along with their photocatalytic and antibacterial applications, was investigated. The natural bentonite (NB) used in this study was purified through acid treatment to obtain activated bentonite (AB). Subsequently, AB was intercalated with Fe^{3+}, resulting in FeAB. TiO_2 and three nanocomposites (TiO_2/NB, TiO_2/AB, and TiO_2/FeAB) were synthesized using sol–gel and hydrothermal processes [1-3]. The materials were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM) combined with energy dispersive spectroscopy (EDS), and the Brunauer-Emmett-Teller (BET) method. SEM images showed significantly larger particle aggregates associated with bentonite and smaller particles corresponding to TiO_2. The TiO_2-pillared clays exhibited superior photocatalytic properties compared to TiO_2 nanoparticles alone for the degradation of Metoprolol tartrate (MET). Among these materials, TiO_2/FeAB proved to be the most efficient photocatalyst. The antibacterial activity of all samples was tested against *Escherichia coli* (Gram-negative) and *Staphylococcus aureus* (Gram-positive) bacteria. Remarkably high bacterial inactivation was achieved within 1 hour of visible light irradiation for *E. coli*, while in the dark, all *S. aureus* colonies were eradicated within the first 30 minutes.

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Elaboration and characterization of 2% Mn doped ZnO nanoparticles for the elimination of 2-Mercaptobenzothiazole.

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Industrial wastewaters containing 2-mercaptobenzothiazole (MBT), a commonly used chemical additive, are typically unable to be treated successfully using conventional biological methods, posing an environmental danger [1]. There are many studies for the degradation of MBT by photocatalysis method [2].

Our study describes the elaboration of photocatalytic nanoparticles of ZnO doped with 2% Mn by the sol-gel method for the degradation of MBT by the photocatalysis method. The production of the powder is a very important and delicate step; in our case it consists of a succession of steps which result in the formation of ZnO doped with 2% Mn powders. The method used require the preparation of a solution called gel solution, drying it, and finally applying heat treatments to crystallize the powder and form 2% Mn doped ZnO. the nanoparticles have been characterized by X Ray Diffraction. The purpose of the XRD study is to determine the crystal structure of the powders produced, to confirm the formation of the crystal phase and to evaluate the size of the crystallites. The results of XRD shows that the samples have a hexagonal Wurtzite crystal structure, the sizes of which are between 22 and 27 nm. In this study we studied the photocatalytic degradation of an aqueous suspension of 2-Mercaptenbenzothiazol (MBT) as a model pollutant of concentration of 10 mg/l and 1g/l of the semi-conductor. The degradation of the MBT was monitored by the spectrophotometric method. Our results show that the degradation rate of MBT exceeds 92,2% for a period of 180 min.

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Phytochemical Characterization and Assessment of Antioxidant Effect of Algerian *Seseli tortuosum*

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The 20th century was the scene of many studies on new bioactive molecules via the screening of natural resources, which resulted in the discovery of a large number of drugs beneficial for the treatment of much human pathology. Algeria is considered among the countries known for its taxonomic diversity because of its position privileged biogeography, it countains more than 3000 species of plants, 15% of which are endemic.

The Apiaceae family has been known since the ancient Chinese and Indian civilizations of Mexico, as well as the Greeks and Romans. The Apiaceae, formerly called Umbelliferae, are aromatic plants due to their secretionof essential oils. This family is rich in secondary metabolites and comprises coumarins, flavonoids, acetylenic compounds and terpenic lactones [1]. This plant has shown various phytotherapeutic properties.

The present study aimed to evaluate the phytochemical properties and antioxidant activity of the Algerian endemic plant *Seseli tortuosum*, *in vitro.*

HPLC analysis, phytochemical screening, thin layer chromatography, polyphenols and flavonoid contents were conducted to determine the bioactive contents of the Algerian Seseli tortuosum plant. Antioxidant activity was tested using DPPH and ABTS scavenging assays, reducing power, phenanthroline and silver nanoparticle (SNP) assays.

Phytochemical analysis highlighted the richness of the extracts in terms of coumarins, terpenoids and quercetin. The quantitative determination of total polyphenols and flavonoids showed that the highest amounts occurred in the dichloromethane (DCME) and methanolic (MeOH) extracts. The antioxidant activities indicated a moderate potential. Conclusion: This study demonstrated the richness of the phytochemical components of seseli tortuosum, which are responsible for several biological properties.

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Structural, Spectral and Hirshfeld Surface Analysis of a Novel Fe (II) Coordination Polymer based on cyanopyrazine: Insights into Magnetic behavior and Catalytic Activity

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In recent decades, coordination polymers (CPs) have gained significant attention due to their diverse architectures and the growing demand for functional materials with tuneable properties (Zahedi, 2018). CPs have potential applications in various fields, like catalysis, biological applications and in optical, magnetic, and electronic devices (Hao, 2015). Several factors influence the structure and properties of CPs, including the oxidation state and coordination geometry of metal centre and the structural chemistry of organic spacers. Additionally, weak interactions such as hydrogen bonding, π–π stacking play a crucial role in controlling the network (Souri, 2018). Magnetic molecular materials have become widely studied due to the need to understand magnetic interactions between paramagnetic ions, bridged by ligands, to develop magneto-structural correlations and their applications in molecular data storage (Liu, 2015). Metal-catalysed epoxidation of olefins is a crucial process in chemistry, widely used in modern organic synthesis, pharmaceutical production, and the creation of monomers for bulk polymers. Iron-based catalysts, particularly those with nitrogen donor ligands, have shown remarkable efficiency in the epoxidation of olefins over the past decade, achieving excellent results in improving the selectivity and activity of the reaction (Perandones, 2013).

An attempt was made in this work to synthesize a CP with interesting structure and profitable properties. Hence, New Fe (II) coordination polymer $[Fe(Pz\text{-}CN\text{-}\kappa N)_2(\mu\text{-}Pz\text{-}CN)_2(NCS)_2]n$ was synthesized using a neutral rigid bidentate N-donor ligand, cyanopyrazine (Pz-CN). Structural characterization of compound was carried out by infrared spectroscopy and the crystal structure was confirmed by single crystal x-ray diffraction method. The x-ray analyses demonstrate that the CP crystallizes in the monoclinic system with P21/n space group. The Fe (II) cation have a hexacoordinated environment forming FeN_6 distorted octahedron geometry around itself (Fig 1). The structure of iron (II) complex is a one-dimensional zigzag chain extended along [101] axe. The development of 2D network is assured by non-coordinated nitrile group on the Pz-CN ligand and S atom of isothiocyanate co-ligand which are engaged in H-bonding interactions with C−H aromatic groups of pyrazine ring. The 3D network is stabilized by π···π stacking and C−H···π interactions. A Hirshfeld surface analysis was performed indicating a significant contribution from N…H/H…N (26.3%), N…C/C…N (16.7%),S…C/C…S(13.7%),S…H/H…S(13.1%),C…H/H…C(8.3%),H…H(6.7%)interactios, among others. Moreover, the magnetic measurements of the material were performed by temperature depends of the magnetic susceptibility (Fig 2). $[Fe(Pz\text{-}CN)_4(NCS)_2]n$ play a magnetic phase transition in the temperature range. Finally, the catalytic activity of this iron

complex has been judged as an efficient catalyst for the oxidation of trans-Stilbene (Scheme 1). A variety of reaction conditions like temperature, oxidant was thoroughly studied to optimize the media of oxidation.

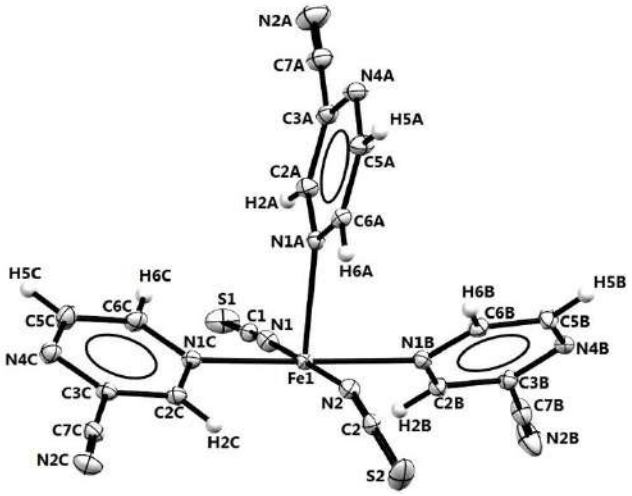


Figure 1 The asymmetric unit of coordination polymer.

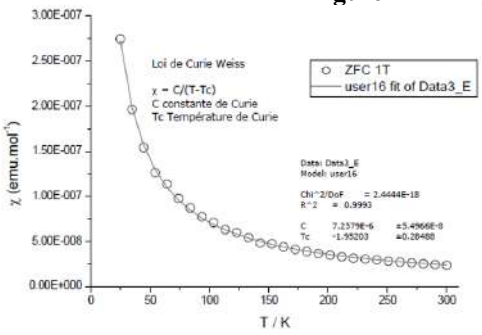
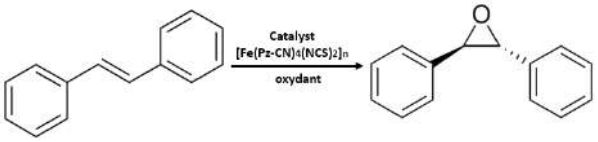


Figure 2 Temperature dependence of the magnetic susceptibility measured at H = 1T



Scheme 1 oxidation of trans-Stilbene

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Synthesis and characterization of two ligands of 1-(diazenyl)naphthalen-2-ol derivatives

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In this study, we report the synthesis and characterization of two ligands of 1-(diazenyl) naphthalen-2-ol derivatives, using the classical method of synthesis, coupling β-naphthol with diazonium salts derived from aniline. Physiochemical properties of the synthesized compounds were determined by their melting points, FTIR, ^{1}H-NMR, ^{13}C-NMR, and Single-crystal X-ray diffraction.

Analyses results showed that these compounds exist in two tautomeric forms (Azo–Hydrazone), with the hydrazone form being more stable. This comprehensive characterization validated the structural integrity and unique properties of the ligand, highlighting its potential for other chemical applications.

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Naphthyridine Derivatives: Synthesis and Biological Evaluation

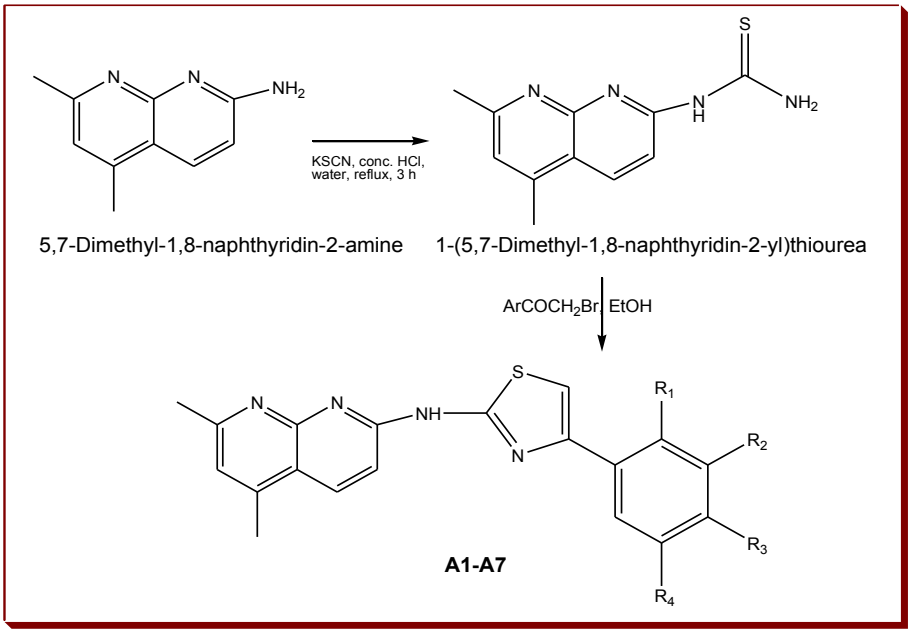
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First, in an acidic environment, the starting material 5,7-dimethyl-1,8-naphthyridin-2-amine interacted with potassium thiocyanate, and then α-bromoacetophenone was added. Six distinct Gram (+) and Gram (-) standard human pathogenic bacterial strains were used in the in vitro CLSI microdilution antibacterial evaluation that followed the production of the novel 7 naphthyridine derivatives. The compound 4-(2,5-Dimethoxyphenyl)-N-(5,7-dimethyl-1,8-naphthyridin-2-yl)thiazol-2-amine was the most significant derivative against the tested bacteria, according to the preliminary results (MIC 0.0625-0.25 mg/mL), with a particular susceptibility to Bacillus subtilis, Staphylococcus aureus, and S. epidermidis [1-2].

The chemical N-(5,7-Dimethyl-1,8-naphthyridin-2-yl)-4-(3-nitrophenyl)thiazol-2-amine, interestingly, exhibited modest inhibitory efficacy against the same pathogens as well (MIC 0.25 mg/mL). The chemicals inhibited Salmonella typhimurium, Listeria monocytogenes, and Enterobacter aerogenes, the remaining human pathogens, by amounts greater than 2 mg/mL. There is still a need for more thorough testing against various diseases [3].



Scheme 1. The synthetic route for the preparation of the derivatives (A1-A7).

Keywords: Naphthyridine, antibacterial, in vitro, MIC, Gram (+), Gram (-).

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Nouvelle procédures de synthèse des dérives de 2- azapyrrolizidine catalysée par Peridiniume para toluène sulfonate (PPTS)

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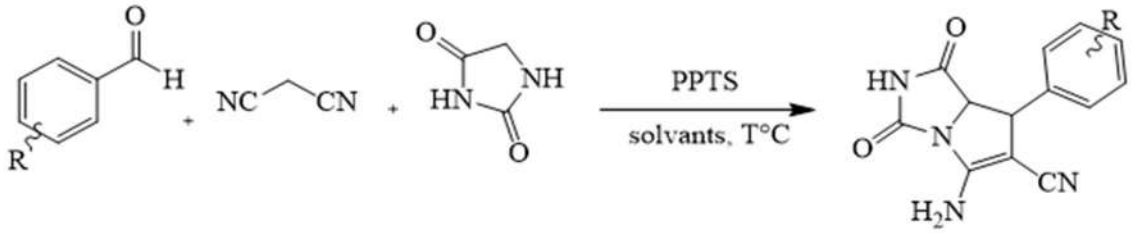
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L'hydantoïne (nom IUPAC: imidazolidine-2,4-dione) est un dérivé d'imidazole hétérocyclique saturé (système hétérocyclique). Il a deux fonctions lactames (amides cycliques),(1) ce qui se produit relativement rarement dans la nature. Le produit naturel le plus connu avec le cycle hydantoïne est le dérivé d'urée allantoïne.(2)

Les imidazolidine-2,4-diones ou d'hydantoïnes(3) sont utilisées dans plusieurs types de synthèse organique actuellement et dans la préparation de beaucoup d'analogues(4). Elles présentent diverses propriétés pharmacologiques intéressantes et occupent une place importante dans la recherche de médicaments car elles possèdent des propriétés anti-ulcère, antitumorale, antivirale, anti androgène, antimicrobienne, antihypertensive, anti-diabétique, antiarythmique, anticonvulsion, anti androgénique et anti VIH(5), antifongique, antibactérienne et antiinflammatoire. Eles sont utilisés dans le traitement de l'hypoglycémie, ou comme inhibiteurs de la croissance des plantes. (3)

Les meilleures activités pharmacologiques ont été réalisées avec des dérivés d'hydantoïne: la phénytoïne comme antiépileptique, de l'azimilide comme antiarythmique, de la Nitrofurantoïne comme substance antibactérienne ou du dantrium comme relaxant des muscles squelettiques; de plus, les hydantoïnes ont également été développées en tant que nouveaux médicaments dans le traitement d'autres maladies, par exemple le nilutamide, un anti androgène actif par voie orale dans le traitement du cancer de la prostate métastatique. (6)

La synthèse des dérivés 2-azapyrrolizidine par une condensation de knoevenagel entre l'hydantoïne (l'imidazolidine-2,4-dione) et une diversité d'aldéhydes (aromatiques, hétéroaromatiques…) et la malononitrile, catalysée pour la première fois par le peridinium para toluéne sulfonate (PPTS). La réaction a été effectuée dans des conditions exemptes de solvant.



Mots clés: l'imidazolidine-2,4-dione, 2-azapyrrolizidine, Knoevenagel, peridinium para toluéne sulfonate (PPTS).

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Use of Urtica Dioica as biocoagulant for wastewater treatment: optimization by box-Behnken design

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In an era when the world is moving towards green technologies to preserve human health in particular and the planet in general, the use of chemicals coagulants, and permeable materials in wastewater treatment is a hindrance, due to their limitation and the dangerous effects on the ecosystem. Therefore, the use and exploration of natural coagulants in wastewater treatment could reduce and exclude the damage implied by chemical coagulants and promote an alternative approach toward a sustainable environment [1].

This study investigates the potential of Nettle (Urtica dioica) leaves as a natural biocoagulant for the removal of turbidity and total suspended solids (TSS) from industrial wastewater, addressing the limitations and environmental impacts associated with conventional chemical coagulants. The surface functionality and surface charge of the powdered Urtica Dioica leaves was studied using FTIR and pHpzc, respectively. Employing a two-step optimization methodology, initial jar tests qualitatively assessed coagulation and flocculation efficacy, followed by Response Surface Methodology (RSM) using Box–Behnken Design (BBD) to quantitatively evaluate interactions among critical operational parameters. The research focused on three independent variables: stirring speed (X1), coagulant dosage (X2), and flocculation time (X3), while measuring the dependent variables of turbidity removal efficiency (Y1) and TSS removal efficiency (Y2).

The results demonstrated that Nettle leaves can achieve significant removal efficiencies under optimal conditions, with a TSS removal efficiency of 96.46% at a coagulant dosage of 1 mL/L, stirring speed of 50 rpm, and flocculation time of 15 minutes, while turbidity removal reached an impressive 99.17% at the same dosage but with an optimal stirring speed of approximately 56.06 rpm over 15 minutes.

These findings underscore the effectiveness of Nettle leaves as a sustainable alternative to chemical coagulants in wastewater treatment processes, highlighting their ability to significantly mitigate turbidity and TSS, thereby improving water quality. This research aligns with broader environmental sustainability goals by reducing reliance on synthetic chemicals and emphasizes the importance of exploring natural coagulants in addressing pressing environmental challenges associated with wastewater management. Ultimately, the study concludes that Nettle leaves represent a viable and eco-friendly solution for wastewater treatment in industrial contexts, suggesting further research to explore the scalability and long-term effectiveness of Nettle-based treatments across various wastewater applications.

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Application for Drinking Water and Wastewater Treatment and Its Potential for Sludge Recovery. International Journal of Environmental Research and Public Health.; 17(24):9312.

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Rapid Fabrication of $(Ba_{0.95}Ca_{0.05})(Sn_{0.10}Ti_{0.90})O_3$ (BCST) Ceramics via Reactive Flash Sintering

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In this study, $(Ba_{0.95}Ca_{0.05})(Sn_{0.10}Ti_{0.90})O_3$ (BCST) ceramics, recognized for their promising dielectric and piezoelectric properties, were explored. Traditionally, the manufacturing process of these ceramics is long and energy-intensive, typically requiring high sintering temperatures (~1500°C) and extended preparation stages, which often limit the control over grain size and overall material performance [1-3]. To address these limitations, BCST ceramics were synthesized using the reactive flash sintering (RFS) technique, which offers a more efficient approach [4]. In this method, a precursor mixture of $BaCO_3$, $CaCO_3$, SnO_2, and TiO_2 powders was subjected to sintering at a lower temperature of 1100°C for a significantly reduced duration of just 10 minutes. During the RFS process, an electric field with a strength of 150 V/cm and a current density of 40 $mA.mm^{-2}$ were applied to facilitate the sintering process. Remarkably, a single-phase perovskite BCST structure was successfully formed within the short sintering time of 10 minutes.

Various characterization techniques were employed to evaluate the structural, microstructural, and dielectric properties of the synthesized BCST ceramics. The use of RFS not only reduced the required sintering temperature and time but also allowed for precise control over the grain size. This resulted in ceramics with refined grains and high density, which in turn contributed to the enhancement of their electrical properties. The combination of grain refinement and optimized density achieved through RFS provided significant improvements in the dielectric performance of the BCST ceramics, making this method a promising alternative for the efficient fabrication of high-performance dielectric materials.

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Electronic tuning effect of auxiliary ligand X on the redox properties of pentavalent biscyclopentadienyl-uranium complexes Cp2UV(=N-Ar)X. STUDY OF DFT / ZORA RELATIVISTE.

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Abstract :

In this work, we present a relativistic DFT study of a family of uranium complexes Cp2U(=N-Ar)X, ($U^{VI}/U^{V}/U^{VI}$), associated with functionalized ligands X type σ and / or π donor. These compounds, whose X-ray structure of some of them is known, have not been the subject of any theoretical study to date. We will particularly study molecular geometries, the relationship between electronic structure and redox behavior and the nature of the metal-ligand interactions involved. We will analyze the different possible correlations between the values of the calculated quantum quantities (EA, IE, net metal charge, HOMO/LUMO and bond indices) with the variations of the half-wave redox potential (-E1/2) measured experimentally. As part of the predictive aspet of the DFT method, we will analyze the redox properties of some unknown or not yet isolated species. These series, were synthesized by the group of Kiplinger et al, and whose X-ray structures and electrochemical data, are known for most compounds .

The DFT calculation method used is based on the ZORA/COSMO+SO approach conducted using the ADF code. Relativistic calculations, taking into account solvent effects and spin-orbit coupling, led to a good correlation AE(eV) vs. -E1/2 (V) with a factor $R2 > 0.97$ in good agreement with the bibliographic data, testifying to the robust model used.

Keywords :Redox potential, Electronic affinity, DFT/ZORA .

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Synthesis and characterization of a new series of magnetic molecules based on lanthanides ions (III)

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Introduction

Lanthanide ions have been widely used in the design of magnetic molecules[1], due to their slow relaxation of magnetization which continue to fascinate the molecular magnetism community since the discovery of such characteristics in a mononuclear terbium phtalocyanine complex more twenty years ago[2]. Such functional molecular systems are often referred as potential candidates for technological applications spanning from quantum computing to high-density data storage.[1,3] Recent progress in the field of lanthanide SMM has led to systems exhibiting magnetic bistability a few kelvins below liquid nitrogen boiling temperature, confirming their great potentiality.[4,5]

Important efforts have been made to deeply understand the parameters affecting the relaxation dynamics in order to ultimately optimize the SMM.[6]

Following this, we report the synthesis, structures and magnetic investigations of a series of new dinuclear complexes based on 2-ethoxy- cinnamic acid. This ligand was chosen to see the influence of changing the nature of the substituent on the coordination environment around the lanthanide sites (symmetry), as well as on the packing arrangement and magnetic behavior.[7]

Experimental procedures

Synthesis of $[Ln(L)_3(DMSO)_x(DMF)_y(H_2O)]_2$. (Ln= Gd (1), Dy (2) and Er(3)) 2-Ethoxycinnamic acid (0.3 mmol) and sodium hydroxide (0.3 mmol) were dissolved in a mixture of DMF:water (2:1). After several minutes of stirring $Ln(NO_3)_3 \cdot 6H_2O$ (,0.1 mmol) was added, and then a yellow precipitate appeared. The precipitate was filtered and recrystallized in DMSO. The resulting solution was allowed to evaporate slowly in an open atmosphere. After a few days, colourless crystals suitable for X-ray analysis were obtained, filtered and dried in air.[8]

Results and discussions

We report in this poster the synthesis, structures and magnetic investigations of a series of new dinuclear complexes based on 2-ethoxy- cinnamic acid (Scheme 1). The dinuclear complexes of the respective formulas $[Ln(L)_3(DMSO)(H_2O)]_2$ (Ln = Gd (1), Dy (2) and Er(3)) were obtained by the reaction between 2-ethoxy-cinnamic acid (L) (3eq) and $Ln(NO_3)_3 \cdot 6H_2O$ (1eq) in a H_2O/ DMF/DMSO. Colorless crystals of the three complexes were obtained by slow evaporation of the reaction mixture at room temperature after a few days.

For all compounds, the asymmetric unit consists of one crystallographically independent Ln^{3+} ion and three deprotonated L^{-} ligands. The two Ln^{3+} ions are connected by six oxygens belonging to carboxylate moieties giving a centrosymmetric dinuclear unit. One water molecule and one coordinated solvate, disordered DMSO/DMF with a different occupancy rate for 1, 2, and 3 complete the coordination sphere to give a coordination number of nine (Fig. 1).

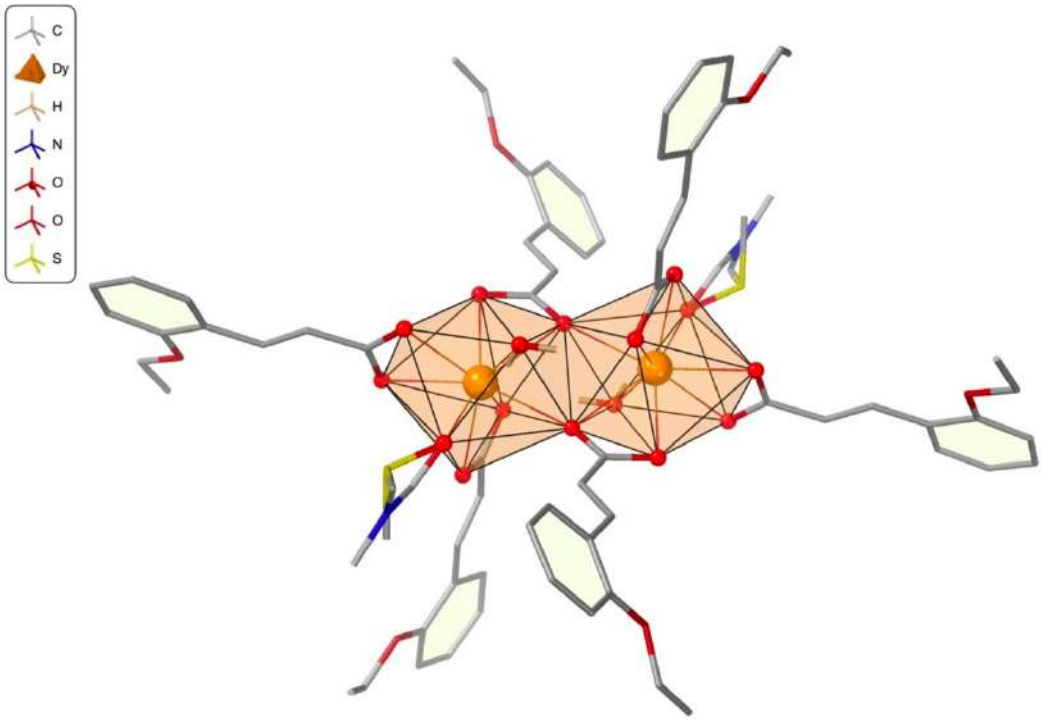


Fig 1: Structure of the dinuclear complexes (1,2 & 3). Hydrogen atoms are omitted for clarity.

Conclusion

Three new lanthanide complexes with a dinuclear structure based on the 2-ethoxycinnamate derivative were synthesized and structurally characterized. The dynamic behaviour of all compounds was then investigated by alternate current (ac) magnetometry in order to probe the occurrence of a slow relaxation of the magnetization. only the dysprosium analogue (complex 2) exhibits a zero-field slow relaxation of the magnetization, A field- induced slow relaxation of the magnetization is observed for compound 1 based on the isotropic Gd^{3+} analogue.

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Green synthesis of reduced graphene oxide nanosheets and assessment of its antioxydant properties

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Reduced graphene oxide (r-GO) has gained significant attention in recent years due to its exceptional properties and versatility in various fields [1]. The synthesis of r-GO usually involves toxic reducing agents that are harmful to human health and the environment [2]. In this study, we report, for the first time, a facile approach for effective reduction of GO using satureja calamintha L. extracts as a green and natural reducing agent.

The GO graphene oxide was obtained by exfoliation and oxidation of graphite by using a modified Hummer's method [3]. In brief, 2g of graphite powder was mixed with 50 ml of H_2SO_4 and stirred for 30 min at room temperature, and then 6g of $KMnO_4$ was slowly added to the suspension under vigorous agitation in an ice-bath and stirred for 2 hours. Then 100 ml of distilled water (DW) was slowly added and 200 ml DW was added instantly. To stop the reaction a 10 ml of H_2O_2 was slowly added to the solution. The obtained solution of GO was washed and dried at 60°C for 2 days.

The reduction of GO was carried out using two extracts, aqueous (Aq) and hydromethanolic (HM), from the plant *satureja calamintha.* The obtained reduced graphene oxide (r-GO) was characterized by using powder X-Ray diffraction (XRD), UV-Vis spectroscopy and Fourier Transform Infrared (FTIR) spectroscopy.

The total phenolic content of the extracts of *satureja calamintha* was quantified by using Folin-Ciocalteu method while the method of aluminium chloride was employed for the quantification of total flavonoid content. The results revealed that aqueous extract is richer in phenolic compounds and flavonoids (643.9 µgGAE/mgE, 164µgQE/mgE) than hydromethanolic extract (237.9 µgGAE/mgE , 84.3µgQE/mgE), respectively.

The antioxidant capacity of the extracts and biosynthesized nanosheets (Aq-rGO and HM-rGO) was determined on the basis of their scavenging of the stable DPPH free radical. The obtained results show that both extracts possessed an important antioxidant capacity, the water extract exhibited higher activity (IC_{50} = 0.028µg/ml) compared to the hydromethanolic extract (IC_{50} = 0.044µg/ml). Therefore, the reduced graphene oxide appeared to be less active than the extracts.

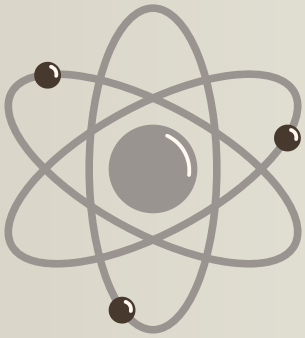
In view of the presence of considerable amounts of antioxidant phytochemicals in *satureja calamintha*, it may act as good reductant for the reduction of GO.

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PHYSICS

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Investigation of Sn-Doping on CuO Nanostructures for photocatalytic Activity

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In this research work, the pure CuO and Sn doped CuO nanoparticles are synthesized by the Sol Gel method for the catalytic property analysis at annealing temperature 400°C for 4 hours. The CuO is being used as a new material because of the ease of availability of raw materials, low cost, non-toxic nature, excellent thermal stability and good optical properties [1]. The unique physical, chemical and optical properties of CuO nanoparticles have numerous potential applications in the fields of photo catalyst [2], batteries [3], gas sensing [4] and solar cells [5].

The structural, optical and photocatalytic properties were characterized by X-ray diffraction study, FTIR spectroscopy, UV–Visible spectroscopy and photoctalytic analysis. The nanopwders X-ray diffraction pattern of pure, Sn doped CuO NPs shows tenorite phase with monoclinic crystal structure, which means that the Sn ions are successfully substituted into CuO matrix. The doping of CuO nanoparticles with 5% Sn improved the crystalline quality by the increase of XRD peaks intensity (Figure.1). The structural parameters shows that the grain size (D) and strain (ζ) increased, while the dislocation density (δ) is decreased (Table.1). Fourier transform infrared spectroscopy studies confirms the functional groups of bonds present in the CuO nanopowders in the synthesized samples (Figure.2).

The optical absorbance decrease by addition of Sn doping indicate that the band gap of CuO NPs is decreased from 1.68 to 1.42 eV (Table.1). Photocatalytic experiments confirmed that our catalysts displayed highly efficient and durable activity for the photodegradation of methylene blue under visible light.The degradation rate of methylene blue (D) of pure CuO fixed at 99.6% after 60 min, but Sn doping importantly reduced the degradation (D) from 99.6 to 10% (Figure.4).

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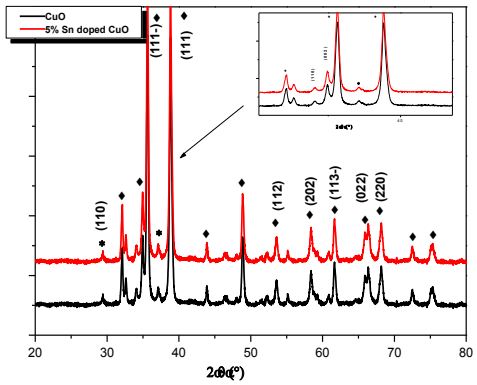


Figure.1 XRD spectre of pure CuO and 5% Sn doped CuO.

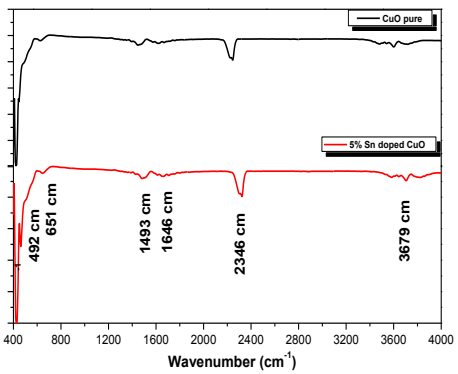
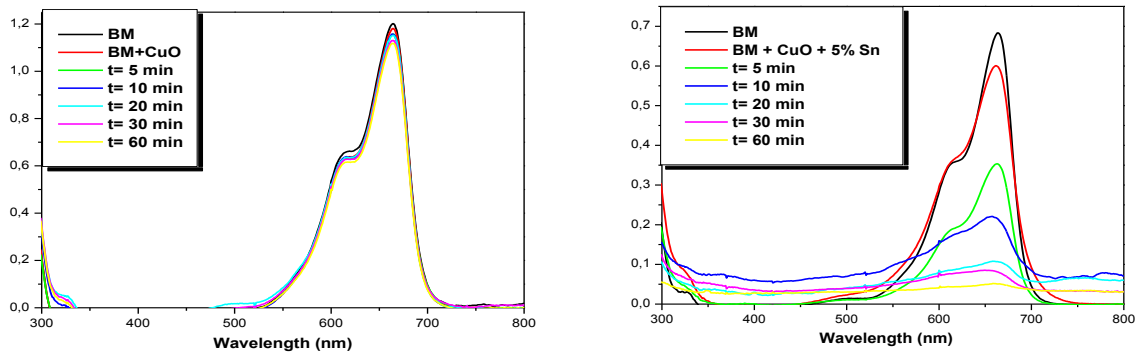


Figure.2 FTIR spectre of pure and 5% Sn doped CuO.

	Annealing Temperature (C°)		(hkl)	D moy (nm)	δ moy (10^{-4})	ε (10^{-4})	Band gap Eg (eV)
	400°C for 4 hours		(110)	α	α	α	α
			(002)	α	α	α	1,68α
			(111)	17,40α	32,43α	57,95α	α
			(111-)	α		α	α
% Sn	400°C for 4 hours		(110)	α	α	α	α
			(002)	α	α	α	1,42α
			(111)	18,58α	30,33α	61,49α	α
			(111-)	α			α

Table 1. Structural parameters of pure and Sn doping CuO NPs.



(a) (b)

Figure.4 BM Degradation as function of time of pure and Sn doped CuO

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FIRST-PRINCIPLES CALCULATIONS OF THE STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF DOPED SnO_2

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Wide band gap semiconductor oxides, such as tin oxide (SnO_2) has attracted extensive attention due to their potential applications in various state-of-the-art optoelectronic devices such as light-emitting diodes, lithium batteries solar cells, gas sensors and photocatalysis [1]. It is also SnO_2 is an important n-type semiconductor with wide band energy (3.6-3.8 eV) categorized by several promising properties for example low electrical resistivity, high optical transparency in the visible region and high chemical stability. These unique properties make it a suitable candidate for transparent conducting electrodes (TCEs) material [2].

SnO_2 is a material that can be easily doped with a variety of impurities, and it was shown that the properties of SnO_2 nanostructures can be handled by doping it with adequate impurities [3].Very many impurities for doping SnO_2 thin films have been applied by other researchers such as Fluorine (F), Antimony (Sb), Copper (Cu), Nickel (Ni), Cobalt (Co), etc. According to the literature, SnO_2 doped with metallic elements could give rise to the ideal electronic device where the crystallinity, electrical conductivity and optical properties of doped SnO_2 are improved compared to undoped [4].

The objective of this work is to study the influence of doping of cesium on the structural, electronic and optical properties of tin dioxide (SnO_2).The first-principles density functional theory (DFT) calculations are performed using the full potential-linearized augmented plane wave method (FP-LAPW) implemented in the code WIEN2K in order to investigate the effect of doping element on the structural, optical and electrical properties of SnO_2.

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A DFT exploration of structural, electronic, elastic, optical and thermoelectric properties of YTiReZ (Z = Si, Sn) Yttrium based quaternary Heusler alloys for photovoltaic and thermoelectric applications.

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In the present work, we performed calculations to predict the structural, electronic, elastic, optical and thermoelectric properties of yttrium-based quaternary Heusler alloys, YTaReZ (Z = Al, In), using density functional theory (DFT) **[1]**. These calculations were executed using Full-Potential Linearized Augmented Plane Waves (FP-LAPW) **[2]** implemented in the Wien2k code **[3]**, with both Generalized Gradient Approximation (GGA) **[4]** and the hybrid functional (HSE06) approximations **[5]**. The YTiReZ compound crystallizes in the LiMgPdSn-type FCC cubic crystal structure with a space group of F-43m, exhibiting three different phases depending on the atomic arrangements **[6]**. The most stable phase was determined through volume optimization calculations. Both compounds crystallize in the type I non-magnetic phase. The electronic properties, like the band structure and density of states (DOS), were analyzed, revealing that these compounds exhibit semiconductor behavior with indirect band gaps. Regarding the optical properties, our compounds were found to have good light absorption in the visible range spectrum, making them potential candidates for photovoltaic cells applications. Additionally, we evaluated the thermoelectric parameters using Boltz-TraP 2 code **[7]** .The obtained calculations affirm the promising application of these materials in energy conversion technologies.

Keywords: Quaternary Heusler alloys, FP-LAPW, DFT, Wien2k, GGA, HSE06.

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Structural, Microstructural and Optical Properties Investigation of Cobalt-Substituted $ZnFe_2O_4$ nanoferrites

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Ferrite nanomaterials with the general chemical formula MFe_2O_4 (where M refers to divalent metal cations such as Fe, Ni, Mn, Co, and Zn etc.) have garnered significant interest due to their fascinating properties, making them promising candidates for a wide range of applications in electronics, medicine, catalysis, telecommunications, data storage, and gas sensors [1]. Zinc nano-Ferrites are intriguing materials that possess unique properties, including mechanical hardness, excellent chemical stability, energy transfer efficiency, high electrical resistivity, low eddy current loss, and magneto-optical behaviour [2]. These features make them particularly suitable for technological applications that require minimal losses. To enhance the practical applications of these materials and improve their performance doping them with transition metals is a common and effective option.

In this study, we investigated the impact of cobalt substitution on the tetrahedral sites in spinel ferrites $ZnFe_2O_4$, focusing on their structural, microstructural, and optical properties at room temperature. $Zn_{1-x}Co_xFe_2O_4$ (x = 0.0, 0.3) nanoparticles were synthesized using the sol-gel auto-combustion process. X-ray diffraction (XRD) analysis revealed that both compounds crystallized in a single cubic phase with $Fd\bar{3}m$ space group. Shrinkage of the lattice parameter from 8.4460 Å to 8.4318 Å was observed with cobalt substitution. The Raman spectroscopy showed structural disorder caused by Co^{2+} doping. The broadening of the A_{1g} mode attributed to the contributions of Zn^{2+}, Co^{2+}, and Fe^{3+} ions in the same symmetry. X-ray Photoelectron Spectroscopy (XPS) results confirmed the elemental composition and oxidation states of the elements Co, Fe and Zn. Scanning Electron Microscopy (SEM) micrographs displayed a spherical morphology for the synthesized nanoparticles; their average grain size is varying from 42 to 45 nm. UV-Visible spectrophotometry demonstrated a decrease in band gap energy with cobalt incorporation, thereby the photocatalytic efficacy of the $Zn_{1-x}Co_xFe_2O_4$ nanoferrites will be enhanced.

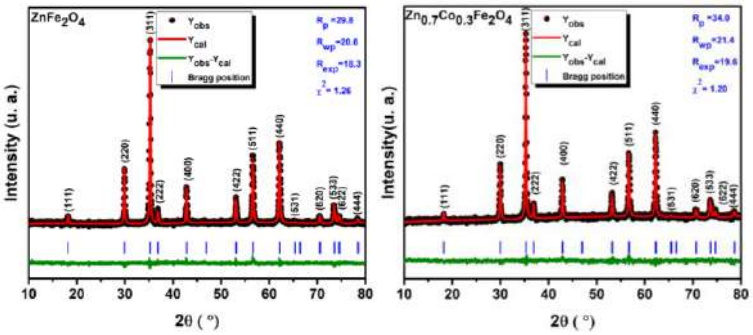


Fig. 1 Rietveld refinement plot of $Zn_{1-x}Co_xFe_2O_4$ compounds

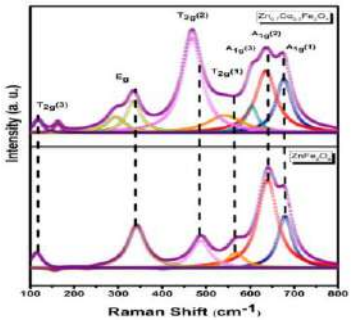


Fig. 2 Deconvoluted Raman spectra of $Zn_{1-x}Co_xFe_2O_4$ compounds.

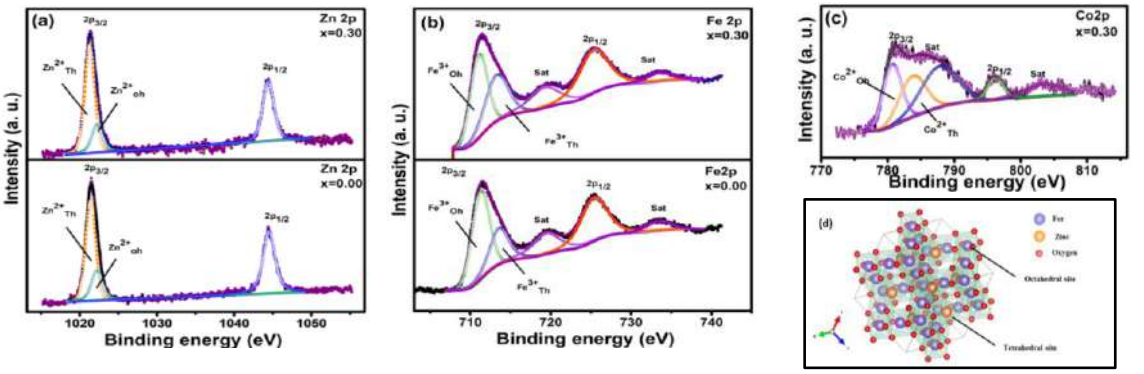


Fig. 3 High resolution XPS spectra and deconvolution of **(a)** Zn2p, **(b)** Fe2p and **(c)** Co2p peak for $Zn_{1-x}Co_xFe_2O_4$ compounds **(d)** Unit cell crystal structure of $ZnFe_2O_4$

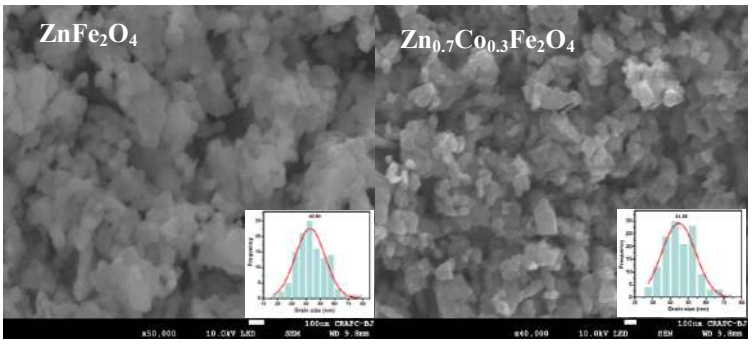


Fig. 4 SEM micrographs of $Zn_{1-x}Co_xFe_2O_4$ compounds

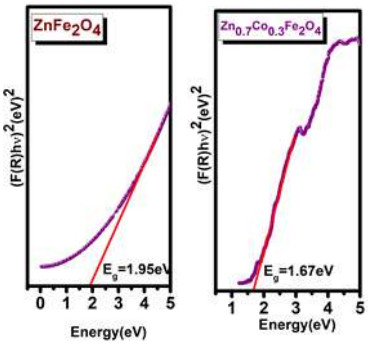


Fig. 5 Plot of $(F(h\upsilon))^2$ versus hυ for $Zn_{1-x}Co_xFe_2O_4$ compounds

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The First International Congress on Recent Advances
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The Schrödinger equation for the pseudo harmonic potential in non commutative space

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Abstract

In this work, we have study of the exact solution of the Schrödinger equation for the pseudo harmonic potential in non-commutative space. The exact energy eigenvalues and the wave functions are calculated by Nikiforov_Uvarov method, then we use the first-order perturbation theory to calculate the correction of energy due to non-commutativity. Finally, we show that the degeneracy of the initial spectral line is broken in transition from commutative space to non-commutative space.

Keywords: Pseudo harmonic potential, Schrödinger equation, Nikiforov_Uvarov method, Perturbation theory; Noncommutative space.

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The First International Congress on Recent Advances
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Optimisation and performance of solar system study using thermal storage

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The main challenge of the energy transition (less expensive and more ecological alternative energy solutions for the production and consumption of energy) is to make current renewable energy systems more sustainable. This change in energy systems is accompanied by an increased need for storage of renewable energy for the supply of electricity, heat and cold. More generally, energy storage is interesting in the areas of network extension or regulation of production peaks. Not to mention the fact that in terms of efficiency, storage is interesting because it allows above all not to waste energy that is already available. [1]

Thermal energy storage is defined as the temporary storage of energy by heating or cooling so that the stored energy can be used later for electricity production, thermal storage provides the essential flexibility to integrate high shares of solar energy into new energy systems. [2]

This study is composed of a 1kw photovoltaic generator and a diesel generator, a converter to convert direct current to alternating current. The energy produced by the system is used for the consumption of a boiler, for simulation results, we use Homer pro software.

The results obtained shows the good performance of the system and the energy storage can help provide constant energy when integrating renewable energy sources with a fluctuating supply. The major drawback of renewable energy and mainly solar energy is that it is an intermittent source (night, sun obscured by clouds).

More generally. The solution is therefore to store the heat produced by solar energy to meet energy needs when and where they arise. Once the thermal energy is collected by solar collectors (flat, parabolic, hyperbolic, mirror) it must be stored efficiently for later use. [2]

Therefore, it is of great importance to design an efficient energy storage system, and the prospects for using such systems are promising because they allow a better use of renewable energy resources, for example in combination with the production of heat from solar thermal energy. In the industrial field in particular, thermal storage allows the judicious use of thermal waste and thus serves to improve the overall efficiency of industrial processes. [3]

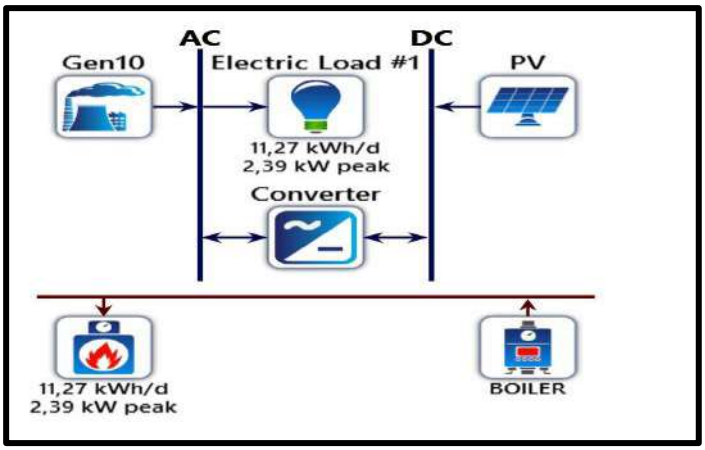


Fig1: Schematic of the proposed system

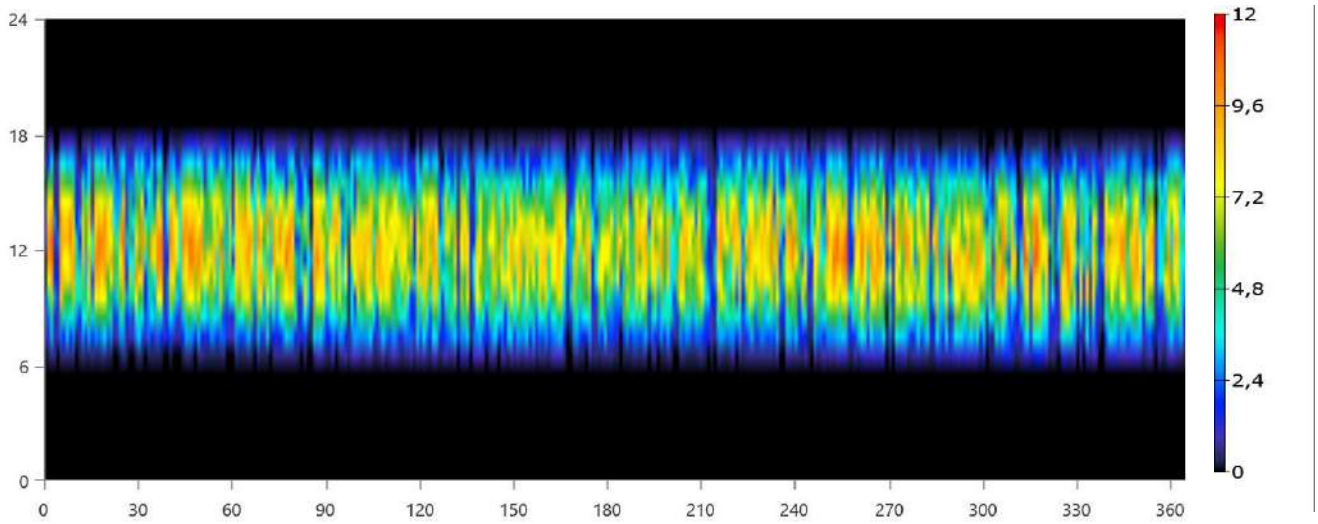


Fig 2: Generic flat plate PV Output (kW)

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The First International Congress on Recent Advances in Mathematical,
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Crystal Structure, Hirshfeld Surface Analysis, Interaction Energy, Energy Framework, Crystal Void, and Theoretical Investigations: DFT and Docking of (E)-1-[-2-(4-Chlorophenyl)Diazan-1-ylidene]Naphthalen-2(1H)-one

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Abstract

(E)-1-[2-(4-chlorophenyl) diazan-1-ylidene] naphthalen-2(1H)-one (4-ClPDN) is an organic compound from the azo dye family.

Its structure was characterized using single-crystal X-ray diffraction (XRD). To explore the intermolecular interactions within the crystal, Hirshfeld surface (HS) analysis was performed using CrystalExplorer [1]. Additionally, interaction energy and energy frameworks were employed to examine the cooperative effects of these interactions throughout the crystal. Crystal voids were also analyzed with CrystalExplorer [1] to gain deeper insights into crystal packing.

Density Functional Theory (DFT) calculations were performed using Gaussian 09W [2], to determine bond lengths, angles, and the molecular planarity of 4-ClPDN. These calculated values were compared with experimental data obtained from X-ray diffraction studies, revealing a close match between theoretical and experimental results, indicating that the DFT calculations accurately reflect the molecular structure.

DFT also provided insights into the electrostatic potential (ESP), and visualized the Highest Occupied Molecular Orbital (HOMO)-Lowest Unoccupied Molecular Orbital (LUMO) distribution, non-covalent interactions (NCI), localized orbital locator (LOL), and electron localization function (ELF), using VMD Studio [3] and Multiwfn [4] for visualization.

Molecular target prediction using the SwissTargetPrediction web server [5] identified 11 -hydroxysteroid dehydrogenase 1 (11 -HSD1) as a probable target for 4-ClPDN. Molecular docking studies were conducted to assess its potential inhibitory activity against 11 -HSD1.

Keywords: XRD, DFT, Docking, Hirshfeld.

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The First International Congress on Recent Advances
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Simulation of an SPR detector for biogas detection based on a heterogeneous metal nanolayer using T-Matrix

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Surface plasmon resonance (SPR) is a pioneering technique in optical sensors that has gained widespread interest and is used in various applications such as biosensing, solar energy, and detection of gases such as hydrogen gas and biogas, being an efficient and renewable source. This paper presents a simulation of the structural response of multilayer surface plasmon resonance and detection by spectral interrogation in the visible and near-infrared range based on MATLAB and the transfer matrix method (T-Matrix), In this work, a surface plasmon resonance (SPR) sensor is proposed for biogas detection consisting of three different layers, the first layer is a dielectric with a refractive index of na, followed by a heterogeneous metallic Nanolayer with a refractive index of neff, and the third layer is the biogas detection region with a refractive index of nb. In this work, we used aluminium (Al) metal to excite the surface plasmon resonance, The results obtained indicate that the (SPR) effect is present in all reflection curves with a change in the resonance wavelength from 822[nm] to 841[nm]. This shift in the resonance wavelength indicates that the proposed sensor can detect changes in the refractive index of the biogas detection region. We also note that the response of the proposed sensor to Aluminium (Al) metal is almost linear with a good sensitivity of S = 599[nm /RIU]. All these results lead us to conclude that the sensor works well with metal nanostructures with good sensitivity and is therefore considered a good choice for biogas detection.

Keywords: Surface plasmon resonance, biogas, T-Matrix

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The First International Congress on Recent Advances
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Influence of synthesis methods on structural and morphological properties of magnetite nanoparticles: A comparative study of precipitation and solvothermal techniques.

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Magnetite Fe_3O_4 nanoparticles have been highly desired for a wide range of applications due to their unique properties, which are dictated by the shape, size, and structural arrangement of their constituents. In fact, the morphology of these nanoparticles plays a crucial role in determining their functional characteristics. Particular emphasis has been placed on the morphology, structure and purity of magnetite synthesised under various conditions (temperature, pH and reaction time) using two techniques: precipitation and solvothermal synthesis. Scanning electron microscopy (SEM) analysis show that the synthesis method can modify the morphology of nanoparticles. Thus, the nanoparticles synthesised by precipitation have mainly cubic and hexagonal shapes, whereas solvothermal synthesis leads to quasi-spherical morphologies. XRD and Raman spectroscopy results show that the powders are essentially composed of magnetite. However, a slight oxidation of precipitated magnetite to maghemite was observed.

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Natural convection of a nanofluid in a square cavity with an opening

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This study presents a comprehensive numerical investigation of the natural convection phenomenon within a square cavity filled with a copper-water nanofluid. The cavity features an opening centrally located on the right vertical wall. The left vertical wall experiences non-uniform thermal heating, while the remaining surfaces of the enclosure are maintained at a lower, constant temperature. To accurately model this thermal-fluid dynamic scenario, we formulate a mathematical representation of the two-dimensional, steady-state thermal natural convection of laminar flow. This model is expressed in cartesian coordinates and employs the stream-function/vorticity formulation. The resulting system of partial differential equations, along with the corresponding boundary conditions, is solved using an iterative numerical method implemented in FORTRAN, leveraging the finite volume method (FVM). The results indicate an enhancement of heat transfer rates as both nanoparticle volume fraction and opening size increase.

Keywords: Natural convection; Nanofluid; cavity with an opening; finite volume method

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Semi-empirical computation of $K_{\beta 2}$ X-ray fluorescence cross-sections for elements ranging from $_{58}$Ce to $_{92}$U for photon energy of 123.6 keV.

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K-shell X-ray fluorescence cross-sections (XRFCSs) of a wide range of elements at various excitation energies can be established theoretically, experimentally, and analytically. These methods are crucial due to their broad applications in a variety of fields, especially in physical-chemistry, atomic physics and medical research.

This investigation aims to estimate the semi-empirical values of the $K_{\beta 2}$ XRFCSs for elements spanning from $_{58}$Ce to $_{92}$U for photon energy of 123.6 keV. The methodology incorporates using a fitting procedure that involves to interpolate the weighted average values using an analytical function against the atomic number Z and then fitting the ratio $S = \left(\sigma_{K_{\beta 2}}\right)_{Exp} / \left(\sigma_{K_{\beta 2}}\right)_{W}$ employing a second-degree polynomial as a function of atomic number Z. Moreover, the experimental values, alongside their weighted counterparts are gathered from the database collected by [1]. Toward the end, a comparison was made between our results and other experimental values [2,3], highlighting a significant consistency between them.

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preparation of Forsterite Powders

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ABSTRACT

Forsterite is a member of the olivine mineral group and is composed of magnesium, silicon, and oxygen, with the chemical formula Mg_2SiO_4 [1]. This mineral possesses several remarkable properties, including a high melting point of 1890 °C, low dielectric permittivity, minimal thermal expansion, and excellent insulation characteristics, even at elevated temperatures. Consequently, it also demonstrates impressive refractory qualities [2]. Due to its favorable attributes, this mineral plays a role in various industrial applications, including in the manufacture of refractory materials and as a source of magnesium in certain chemical processes.

Various procedures, such as the sol-gel method, sol-gel combustion method, and solid-state reaction, to name just a few, were used to synthesize pure forsterite powder [3]. When comparing these methods with traditional solid-state reaction processes, the latter is considered more straightforward and preferable for large-scale production. However, during the calcination process, the formation of $MgSiO_3$ (a secondary phase) and residual MgO often results in low density, high porosity, poor sinterability, and other inferior properties in the prepared Mg_2SiO_4 products [4]. Traditionally, high-quality minerals such as magnesite, peridotite, serpentinite, talc, and silica are used as raw materials to fabricate forsterite ceramics and other products applied in industry and daily life. The objective of this study is to synthesize forsterite-based ceramics through a solid-state reaction, employing natural silica and magnesium oxide as the initial materials.

KEYWORDS: *Forsterite, Microstructure, DRX, Ceramic powder*

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Characterization of copper thin films synthesized by chemical immersion in several electrolytes of different sodium concentrations

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Nanotechnology is an interdisciplinary field of the sciences of physics, chemistry and materials sciences, meant for the design and fabrication of nanomaterials and their applications. This branch of science is meant to understand the fundamental physical and chemical properties and phenomena of nanomaterials and nanostructures, and because of the novel application of nanomaterials, the science of nanomaterials has evolved as a frontline research area.

There has been a rapid growth in the investigation of nanoparticles and nanocomposites because the properties of nano-scaled particles have attracted the attention of scientists. The term "nanoparticle" is often used to describe particles that show a size of 1-100 nm in at least one of their sizes (width, thickness, length). Particles at this dimension contain only tens to millions of atoms; therefore, the high surface area to volume ratio creates highly active surfaces compared to those bulk materials. Additionally, the energies can be illustrated as being quantized, in which the material behaves in discrete rather than continuous form [1].

The synthesis of nanometal oxide has attracted extensive research interest because of its potential applications in optics, electrics, photocatalysis, gas sensors, information storage, and so forth. It is demonstrated that their properties are determined by their composition.

Among these metal oxides, cuprous oxide (Cu_2O) and cupric oxide (CuO) nanoparticles are particularly interesting not only for the development of synthetic methods but also for the examination of their sensing, photocatalytic, and surface properties. Copper oxide nanostructures have been demonstrated to have properties superior for applications in gas sensing , carbon monoxide oxidation, photocatalysis, soft templates, and organic synthesis [2].

The advantages of copper oxides include their non-toxic nature, the abundance of their precursor materials, and the cost effectiveness of their synthesis routes [3].

The present research work focuses on the synthesis and comprehensive characterization of CuO and Cu_2O nanoparticle thin films fabricated via chemical immersion techniques. The main objective is to investigate the influence of the sodium hydroxide (NaOH) concentration on the structural and morphological properties of the resulting copper oxide thin films. For this, three electrolytes with different concentrations of NaOHwere studied: C1= 2,5M NaOH, C2= 1M NaOH and C3= 0,9M NaOH.

The copper substrates was well polished, then immersed 13 minutes in the prepared solutions at ambient and then treated at different temperatures for 1 hour in the air.The resulting nanostructures of copper oxides were characterized using X-ray diffraction (XRD), Raman and the scanning electron microscope (SEM).

The XRD result revealed that the annealing temperature affects the XRD patterns of the copper oxide films; the intensities of the observed peaks, hence the crystallinity of the thin films, increases with

the annealing temperature. The orthorhombic-structured copper hydroxide $Cu(OH)_2$ was found after immersion in both electrolytes: C1 and C2, and its absence was observed in the electrolyte C3. Also, the monoclinic CuO phase was found in the three studied solutions because of its excellent stability at lower temperatures.

The effect of the concentration of the soda NaOH on the formation of copper oxides was clearly confirmed by Raman spectroscopy. After annealing at 180 °C, the presence of a pure CuO phase was obtained in both thin films after immersing in C1 and C2 and the formation of the cubic Cu_2O phase, in addition to the CuO phase was only observed in the electrolyte C3.

The formation of the cuprous Cu_2O oxide was obtained after annealing at 250 °C in the film immersed in C2 and after annealing at 300 °C in the film immersed in C1.

The formation of Cu_2O depends on the molarity of NaOH. The decrease in the concentration of NaOH decreases the temperature required for the production of Cu_2O copper oxide. The reduction of soda accelerates the formation of Cu_2O.

The crystallite size obtained at different treatment temperatures was calculated by Scherrer relation and the obtained values show that the prepared copper oxide thin films are of the nanometric order.

The surface morphology of the films is improved by annealing the prepared samples in the three studied electrolytes. The increase in the annealing temperature of the copper substrates immersed in the three electrolytes C1, C2 and C3 affects the crystallinity of the layers as well as their morphology. The synthesis of the nanowires and nanoflowers is obtained on the surface of the Cu substrate immersed in C1 and C2 after annealing at 180 °C due to the high concentration of Na ions in basic conditions. However, the lowest concentration of NaOH revealed the morphology of nanofibers and nanoflowers; the nanofiber morphology is highly related to the presence of Cu_2O phase.

The main results show that the formation of Cu_2O depends on the molarity of NaOH. The decrease in the concentration of NaOH decreases the temperature required for the production of Cu_2O copper oxide. The reduction of sodium accelerates the formation of Cu_2O. The increase in the annealing temperature in the three studied electrolytes C1, C2 and C3 affects the crystallinity of the layers as well as their morphology. The structure of nanofibersis strongly linked to the presence of the Cu_2O phase.

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Ab-Initio Investigation of the Electronic, and Thermodynamic Characteristics of Complex Hydrides XAlSiH (X = Sr, Ca, and Ba) for Hydrogen Storage Applications

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Abstract

A comprehensive study utilizing density functional theory (DFT) was conducted to assess the mechanical and thermodynamic properties of polyanionic hydrides XAlSiH (X = Sr, Ca, and Ba). This research marks the first computational analysis of thermal parameters such as the Grüneisen parameter γ, heat capacity, and thermal expansion coefficient for these materials. These parameters were determined using the quasi-harmonic Debye model across a broad range of pressures (0–40 GPa) and temperatures (0–1000 K) [1].

The study revealed varying gravimetric hydrogen storage capacities for BaAlSiH, SrAlSiH, and CaAlSiH, with values of 0.52%, 0.71%, and 1.05%, respectively. Simulations also indicated different hydrogen desorption temperatures for these compounds. Electronic properties were analyzed, showing semiconducting behavior with bandgap values that varied depending on the approximation method used. The study further explored the thermal stability and bonding characteristics of these compounds, highlighting differences in their decomposition temperatures and bonding directions. The findings suggest that these materials exhibit specific thermal behaviors and electronic properties that could be relevant for hydrogen storage applications [1].

Keywords: DFT, Structural properties, Density of states, hydrides compounds, hydrogen storage. Thermodynamic proprieties.

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Investigation of the optoelectronic and thermoelectric properties of Li_2AgAsZ_6(Z=Cl, Br, F) Double Perovskite compounds: First-Principle Calculations.

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In this study, we have investigated a range of structural, electronic, optical, and thermoelectric properties of halide double perovskites Li_2AgAsZ_6 (Z= Cl, Br,F). Our analysis was conducted using the full potential linearized augmented plane wave (FP-LAPW) **[1]** .This particular method relies on the Density Functional Theory (DFT) **[2]** method with the generalized gradient approximation (GGA) **[3]** and the modified Becke–Johnson (mBJ) **[4]** potential. Structural parameters were determined through optimization and analytical schemes, allowing us to precisely define the crystal structure. The electronic properties of these double perovskites reveal their semiconductor nature, characterized by an indirect energy band gap. Optical properties, including as the dielectric function, absorption coefficient, refractive index, extinction coefficient, reflectivity, electron energy loss, and optical conductivity, were computed across a photon energy range up to 13.0 eV to elucidate the optical response of the materials. Additionally, we predicted the thermoelectric properties of Li_2AgAsZ_6 (Z= Cl, Br,F) by calculating key thermoelectric coefficients, including the Seebeck coefficient and power factor were calculated utilizing the Boltz-TraP code**[5]**.Our findings suggest the potential suitability of Li_2AgAsZ_6 (Z= Cl, Br,F)double perovskites for applications in photovoltaic and thermoelectric devices .

Keywords: Double Perovskite, FP-LAPW, DFT, GGA, WIEN2K, BoltzTraP.

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Effects of Adiabatically Trapped Nonthermal Polarization Force on Dressed Dust Acoustic Solitary Waves in Non-Maxwellian Plasma

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The influence of adiabatically trapped nonthermal polarization force on dressed dust acoustic solitary waves (DDASWs) in non-Maxwellian complex plasma is investigated. In particular, we focus our analysis on modifications induced by the Cairns–Gurevich polarization force and higher-order corrections on the main characteristics of the dust acoustic (DA) solitons (DASs). Using the renormalization method, we determined a new solution of the DA solitary waves (DASWs), written as a sum of the *K–dV* solution and the higher-order corrections contribution. Then, we numerically estimated the validity range of the dressed DA wave solutions, with and without the polarization force. Due to this latter force, only lower values of nonthermal parameter α ($\alpha \lesssim 0.11$) are required for the dressed dust acoustic soliton (DDAS) solutions. In addition, we have investigated the impacts of various plasma parameters, namely, the nonthermal parameter α and polarization force R on small-amplitude DDAS. The obtained results show that these parameters play a significant role in modifying the DDASWs. Interestingly, we illustrate that, due to the polarization force and for a fixed value of α, the amplitudes of *K–dV* solitons, higher-order corrections potential, and dressed solitons increase. Furthermore, beyond certain values of α, the higher-order corrections potential becomes rarefactive and consequently, the departure between the *K–dV* amplitude and the dressed dust acoustic (DDA) amplitude becomes more important.

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Synthesis of CuO Nanoparticles using Sol Gel method for photo catalytic application

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Among nanostructured materials of great interest in current material research, copper oxide (CuO) is especially fascinating because of having specific chemical and physical properties which makes it applicable in many areas, such as conversion of energy, optoelectronic devices, and gas sensing [1].

In our work copper oxide nanoparticles are synthesized successfully by Sol Gel method using copper nitrate as a precursor, ethanol as solvent and citric acid as a stabilizing agent. CuO nanoparticles (NPs) were characterized by X-Ray diffraction (XRD), Scanning Electron Microscopy (SEM) and Energy dispersive X-ray fluorescence (XRF), FTIR infrared spectroscopy analysis and by photo catalytic activity using heterogeneous Fenton process. XRD analysis confirmed the monoclinic structure of CuO NPs (figure 1). The obtained lattice parameters a=4.70 Å, b=3.43 Å and c=5.12 Å are in good agreement with those reported in the literature [2,3,4]. SEM image showed spherical morphology of CuO NPs (figure 2), their size being in an order of magnitude less than 100 nanometers. XRF analysis shows two peaks CuKα (8.03 keV) and CuKβ (8.90 keV) characteristic of copper with 98.6% element content (figure 3). The impurities calculated are 1.4%. FTIR spectroscopy confirmed two characteristic bands attributed to Cu-O stretching bands (figure 4). The degradation rate of MB (D) for pure CuO reaches 29.6% after 120 min without H_2O_2. Adding H_2O_2 increases the degradation rate (D) to 97% after 90min (figure 5).

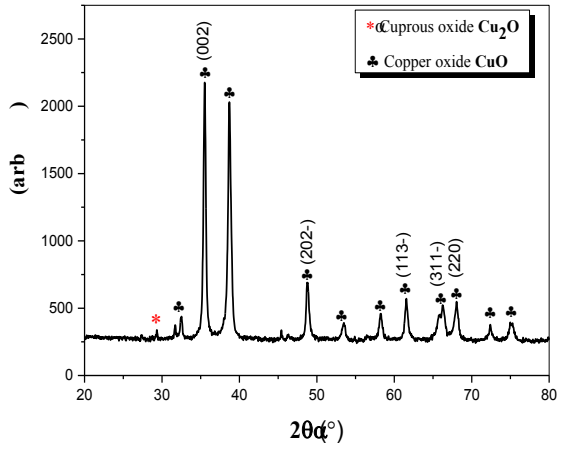


Figure 1: XRD Spectra of pure CuO NPs

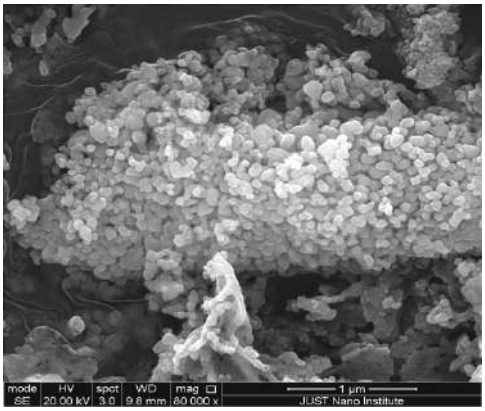


Figure 2: SEM image of pure CuO NPs

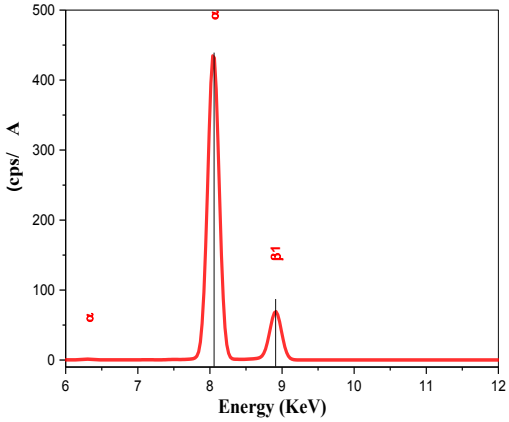


Figure 3: XRF pattern of pure CuO NPs

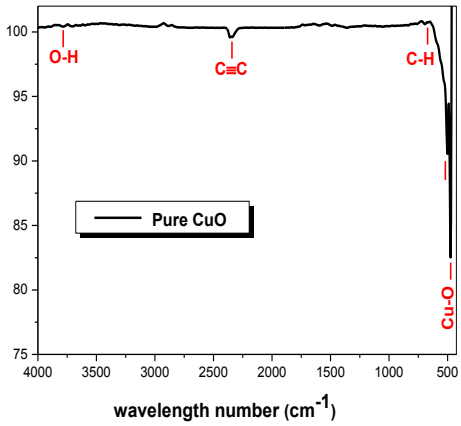


Figure 4: FTIR of pure CuO NPs

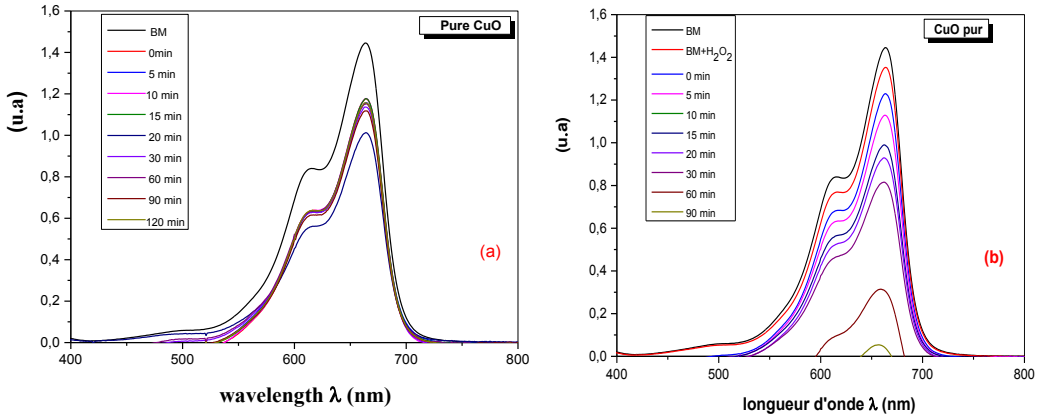


Figure 5: Test photocatalytic : (a) CuO without H_2O_2, b) CuO with H_2O_2

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Preferred presentation format: Poster

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Pressure effect on elastic interaction between dislocation and grain boundaries in Ti-Al alloys

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Abstract

We have studied the elastic dislocation-interface interaction by the Barnett and loth model in Ti-Al alloys, considering an external stress such as pressure. The dislocations having a burgers vector b=a/3[11-20] and the interface characterized by a plane parallel to the dislocation line, and disorientation from 0° to 180° around the axis [0001]. The direction of the image force is related to the anisotropy factor H in the case of dislocation-grain boundary interaction, and by the shear modulus difference (Δμ), in the dislocation-interphase boundary interaction (Ti/ α2). The effect of pressure increases the value of H and Δμ and thus the intensity of the dislocation-interface elastic interaction energy ΔE. The Ti/α2 and α2/α2 interfaces are formed an obstacle for the movement of dislocations. The crystallographic and elastic parameters do not favor the passage of a dislocation located in Titanium to α2 phase. The disorientation of the interface changes the behaviour of dislocations.

Key words: Dislocation; interface; image force; pressure; Ti-Al alloy

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Influence of strain rate on the occurrence of Portevin-Le Chatelierеffect in the Al-2%Mg alloy at room temperature

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In metallic materials loaded at constant driving velocity (hard testing machine), the stress generally varies monotonically and the recorded stress-strain curve is stable. However, for materials subject to the Portevin-Le Chatelier (PLC) effect, such as Al-Mg alloys, plastic instabilities appear on the stress-strain curve. They result from the Dynamic Strain Aging (DSA) mechanism, i.e. from the dynamic interaction between solute atoms and mobile dislocations.

The objective of this study is to characterize the PLC effect in the Al-2%Mg alloy deformed in tension with a hard testing machine at room temperature. It is shown that plastic instability presents a negative strain rate sensitivity of the flow stress. The temporal aspects of the PLC effect depend significantly on the strain and the applied strain rate. Three types of instability patterns (Type A, Type B and Type C) are observed when the applied strain rate decreases and/or the strain increases. Instability parameters, such as the plastic critical strain for instability, the magnitude of the stress drops and the reloaded time between two successive instabilities, are analyzed in accordance of the theoretical models. The obtained results are compared to those reported in the literature.

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Numerical study of the natural convection in tall enclosures usingWater /SiO_2Nanofluid

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This work presents the numerical study of the natural laminar and transient convection in a cubic enclosure filled with nanofluids, having a big horizontal axis, tilted of 45° in relation to the horizontal plane.

The enclosure is filled by a Newtonian and incompressible fluid. Calculations were performed for Grashof number ($10^3 \leq Gr \leq 10^6$) and volume fraction of nanoparticles ($0 \leq \Phi \leq 0.1$).

The SIMPLER algorithm is used for handling the pressure -velocity coupling.We compare results resulting from the latter with other similar results existing in the literature, and validate the model, it is observed from the results that, the average Nusselt number and stream functions increase by increasing the volume fraction of the nanoparticles.

KEYWORDS: Nanofluids, Fluid Mechanic,transient, Heat Transfer, Natural Convection, Closed enclosures

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Spectroscopic properties of isotonic chain N=50 around 90Zr closed core

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Nuclear structure has made great progress in the investigation of nuclei all over the nuclear landscape. Within the shell model framework [1], I will present the energy levels of the isotonic chain N=50 with Z>40. These calculations were performed by using a newly developed effective interaction for the region around 90Zr closed core. This new effective interaction is derived from N3LO realistic interaction, and adapted to the model space by using a low momentum potential approach [2]. The calculated energy levels will be discussed and compared to the experimental data, in order to validate the neutron-neutron two body matrix elements of our effective interaction. The numerical calculations were performed using the Antoine shell model code [1,3].

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Non-commutative Effects in Higgs Boson Pair Production via Z Boson Decay at Electron-Positron Colliders

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Abstract

Particle physics faces significant challenges in explaining phenomena beyond the Standard Model (SM), which motivates the exploration of new theoretical frameworks. Non-commutative geometry offers a promising avenue for extending the SM by introducing modifications to the structure of spacetime at high-energy scales. This theory suggests that spatial and temporal coordinates may not commute at these high energies [1], leading to a non-commutative spacetime. Studying the effects of Non-commutative geometry on particle interactions could reveal new insights into the fundamental nature of spacetime and help explain phenomena beyond the Standard Model. This study investigates the potential signatures of non-commutative geometry in the production of a pair of Higgs bosons (HH) through the process ($e + e- \rightarrow Z \rightarrow HH$) in electron-positron colliders. The event signatures potentially lead to deviations from Standard Model (SM) predictions, offering crucial insights into the nature of spacetime at high energies and shedding light on new physics beyond the Standard Model. Where spacetime coordinates no longer commute according to the usual rules but follow relations such as:

$$[x^\mu, x^\nu] = i\theta^{\mu\nu}$$

The process $e^+e^- \rightarrow Z \rightarrow HH$ was analyzed using techniques from non-commutative quantum field theory. Applying Feynman's rules at order $O(\theta)$ [2]. The cross-section for this reaction was computed and compared to traditional SM predictions. The study found that non-commutative effects can lead to slight deviations in the measured cross-sections when compared to SM predictions. These deviations, while small, could be detectable in future high-precision electron-positron colliders such as the International Linear Collider (ILC) or the Compact Linear Collider (CLIC) [3], which have the potential to provide precise measurements of Higgs-Z interactions.

Keywords: Non-commutative geometry, Non-commutative standard model, Higgs-Z production, scattering cross-section.

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Crystallographic study of molecules which possess biological activities

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To investigate the biological activities of biomolecules, it is essential to study their crystallographic structure, as it is directly related to these activities. The most effective and economical approach involves performing theoretical calculations, followed by experimental analyses to validate the results through various characterization methods.

In this study, we employed Density Functional Theory (DFT), a powerful computational tool that provides key theoretical insights, including molecular optimization, atomic positions, bond angles, and spectra such as NMR and IR.

Using Gaussian software, we performed DFT calculations on the synthesized molecule (E)-1-((1H-inden-2-yl)diazenyl)naphthalen-2-ol. The theoretical results were then compared with experimental data to validate the accuracy of the DFT calculations.

The strong correlation between the theoretical and experimental results demonstrates the reliability of DFT as a predictive tool for studying molecular properties. This approach not only deepens our understanding of the molecular structure and dynamics but also paves the way for further exploration of related biomolecules.

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Numerical investigation of the impact of integrating phase change material into building wall

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Due to substantial population growth in recent decades, the building sector has become the third-largest energy consumer in the world [1]. Moreover, it is responsible for approximately 17% of CO_2 emissions [2]. Air conditioning and ventilation systems are major contributors to this increase. This has prompted the scientific community to explore innovative solutions to save energy. Incorporating phase change materials (PCMs) into building envelopes could be a promising solution due to their ability to store and release latent heat during phase change processes that occur in response to environmental temperature variations [3].

The purpose of this work is to investigate the effect of integrating PCMs into brick cavities on the heat transfer rate in building walls and the role of PCMs in enhancing indoor thermal comfort. This study was carried out using a transient numerical model focused on describing heat transfer in a multi-layer building wall that includes layers of mortar, hollow brick, and plaster. This wall is similar to those installed in most buildings in Algeria. To assess the performance of PCMs, the brick cavities were filled with PCM in two configurations: one close to the interior and the other close to the exterior. The nonlinear governing equations were solved using the finite volume method, and a heat transfer model was developed and solved using computational fluid dynamics (CFD) software. The enthalpy method was employed to simulate the phase change in the PCM.

The results demonstrate that incorporating PCMs into building walls has a noticeable impact on the sinusoidal thermal wave of indoor temperature, primarily due to the phase change phenomenon. This leads to a reduction in heating and cooling needs, thereby confirming the capability of these materials to save energy.

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Synthesis of Silica Nanopowders from Sodium Silicate

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Abstract

Silica (SiO2) is one of the most significant naturally occurring substances utilized in various industrial applications and is a preferred precursor for the production of ceramics due to its abundance and excellent availability. It serves as a fundamental refractory raw material with an ideal composition of SiO2.

In this study, SiO_2 nanopowder was synthesized from sodium silicate. After the drying process, the powder was calcined at temperatures of 600°C and 800°C for one hour. X-ray diffraction (XRD) analysis was employed to identify the phases formed during calcination. The resulting diffraction patterns indicate that the material primarily exhibits an amorphous nature, predominantly composed of SiO2, consistent with existing literature. Notably, calcination at 800°C resulted in the transformation of the amorphous silica into cristobalite, demonstrating the thermal stability and phase transitions of the synthesized material.

This work highlights the potential of sodium silicate as a precursor for producing high-purity silica, paving the way for further research into its applications in advanced materials.

Keywords: Nanopowders; Ceramics; calcination; Silica

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Optimal Dubinin-Astakhov Parameters for Two Bed Adsorption Machine with Mass Recovery Process

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A comparative study of adsorption characteristic parameters of Dubinin-Astakhov equation (characteristic parameter of the adsorbent- adsorbate couple n, the affinity coefficient D, and the maximum adsorption capacity w_0) is presented in this work. Pairs of (AC-35/methanol, silica-gel/water, and zeolite/water) are chosen as working pairs, in order to optimize the performance of two-bed adsorption refrigeration system with mass recovery process. A thermodynamic model was adopted and the adsorption characteristic parameters of the used working pairs were evaluated using Dubinin-Astakhov equation.

The main objective of this work is to develop a thermodynamic model that is able to determine the optimum values of Dubinin-Astakhov parameters for the chosen adsorbent-refrigerant pair.

The performance analysis of the current study obtained using a computer simulation program written in FORTRAN is evaluated by means of cooling power and performance coefficient indicators and parametric analyses have been carried out with various operating temperatures.

The simulation calculation demonstrates that Dubinin-Astakhov parameters of the used couples have a significant influence on the performance's system, and for each couple, there is an optimal value. Furthermore, AC-35/methanol working pair presents good performance for mass recovery process, but it is seriously in competition with the silica gel/water couple which is often preferred due to its ease of implementation and its respect for the environment.

Keywords: Adsorption, Cooling power, Dubinin-Astakhov, Mass recovery, and Performance coefficient.

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Quantum simulation and small molecules: A focus on energy calculation

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Quantum simulation is a technique that emerged as a promising approach for addressing complex problems in physics, chemistry, and materials science. One of the most fundamental properties of molecules is their energy, which governs their stability, reactivity, and spectroscopic properties. The aim of our work is to calculate the energy of the ground and excited states of small molecules (water H_2O and methanimine CH_2NH) using the variational quantum eigensolver (VQE) and the variational quantum deflation (VQD) algorithms.

By encoding the molecular Hamiltonian, a mathematical representation of the molecule's energy, onto the quantum bits (qubits), it becomes possible to evolve the system's quantum state and extract information about its energy levels. The energy calculation process involves several key steps: the first is the Hamiltonian construction, where the molecular Hamiltonian is constructed using quantum chemistry methods, such as Hartree-Fock or density functional theory, to obtain a suitable representation of the electronic interactions. The second step is the qubit encoding, where the Hamiltonian is mapped onto the qubits. The third step is quantum evolution, where the quantum state of the system is evolved under the influence of the Hamiltonian, allowing it to explore the energy landscape. Finally, we perform a measurement and analysis. Measurements are performed on the qubits to extract information about the energy levels of the molecule.

Quantum simulation of small molecules represents a promising avenue for advancing our understanding of chemical processes and materials properties. As quantum hardware and software continue to improve, we can expect to see increasing applications of this technology in fields such as drug discovery and materials design.

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Anisotropic residual stresses in AlN/sapphire epitaxial thin films measured using $\sin^2\psi$ method

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Abstract

Aluminium nitride (AlN) has attracted attention due to its excellent properties. It is generally used as a template for growing AlGaN and GaN heterostructures. In fact, the residual stress generated inside the layers impact the performance of device, especially semiconductor devices like AlN. In our work, we report the structural characterizations using high resolution x-ray diffraction technique (HR-XRD) of AlN films grown on c-axis sapphire substrate by metalorganic vapour-phase epitaxy (MOVPE). Phi scans results was used to confirm the epitaxial growth of AlN layer. Therefore, the $\sin^2\psi$ approach was performed to extract the residual stress components in AlN/sapphire films. The compressive biaxial stress is dominated inside AlN samples at different growth conditions. It was observed that AlN films display an anisotropic behaviour, Consequently, the results obtained show a high anisotropic growth behaviour, this anisotropic in the growth is reflected from the differences of the lattice mismatch values, thermal expansion coefficients and adatom kinetics along the in-plane directions during the growth process.

Key words: Residual stress, AlN, MOVPE-growth, HR-XRD.

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Comparative Study on the Use of Treated and Untreated Olive Husk in Bio-Lightweight Concrete: Effects on Thermal, Mechanical, and Moisture Absorption Properties

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Abstract:

This research explores the use of olive husk, a renewable byproduct of olive oil production, as a sustainable additive in bio-lightweight concrete. This research investigates the use of treated and untreated olive husk as a sustainable additive in the production of a bio-lightweight concrete, assessing its impact on the material's thermal, mechanical, and moisture absorption properties. Olive husk was added to concrete mixtures at 15% by weight, in both treated and untreated form (BLCT15 and BLC15), to evaluate its potential as a substitute for conventional concrete which is represented as the reference sample (BLC0). The findings reveal that both untreated and treated olive husk enhances the thermal performance and increases the porosity of the concrete, leading to lower thermal conductivity and improved insulation capabilities. Both treated and untreated samples (BLCT15 and BLC15) showed an improvement in the moisture absorption capacity compared to the reference samples BLC0, Yet, untreated samples (BLC15) showed a slightly better moisture absorption capacity, as indicated by the sorption isotherms. On the other hand, both treated and untreated OH samples showed a reduction in compressive strength resulting in greater hygrothermal performance while maintaining acceptable mechanical behaviour. However, the reduction was much more pronounced in the untreated OH-based samples. Overall, this research demonstrates that olive husk, both treated and untreated, can be a viable, eco-friendly component for developing building materials with better thermal performance, contributing to more sustainable construction methods.

Keywords:
Olive husk, OH, bio-lightweight concrete, thermal conductivity, porosity, mechanical strength, moisture absorption, resorption isotherms, treated, untreated, sustainable construction, eco-friendly building materials, hygrothermal performance.

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Ultrasoft Scalars Energy at Next to-leading order in Hot Scalar QED

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Abstract

The difficulties encontred in the infrared sector within the gluon and quark damping rates calculated using imaginary time formalism [1, 2, 3, 4, 5, 6, 7]. A similar observation has been done in the context of scalar electrodynamics [8]. To look further into the infrared behavior, we propose to calculate the next-to-leading order dispersion relations for slow-moving Scalars at high temperature scalar quantum electrodynamics (Scalar QED), using the real time formalism (RTF) in physical representation. We derive the analytic expressions of hard thermal loop (HTL) contributions to propagators and vertices to determine the expressions of the effective propagators and vertices in RTF that contribute to the complete next-to leading order contribution of retarded scalars self-energy. The real part of the retarded scalars self-energy is related to the next-to-leading energy of ultrasoft moving scalars.

Keywords*:* Hard thermal loop, Hot Scalar QED, NLO Computations, Ultrasoft moving scalars energy, Infrared divergences

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development and evaluation of maximum power point tracking charge controller in the production of solar technology in remote areas.

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Sustainable energy resources are considered to produce energy without fuel consumption. From there, photovoltaic (PV) is selected due to advantages such as non-pollution and low computational cost. Due to advancements in power systems and smart grids, researchers are interested in developing control systems for renewable energy resources. Solar Charge Controller with Maximum Power Point Tracking is needed to extract maximum energy from photovoltaic.

This study present a photovoltaic system connected with MPPT charge controller installed in Constantine Algeria. The experimental results shows the effect of MPPT controller in the potential and the production in solar system, And the satisfactory performance of MPPT charge controller in terms converter efficiency, MPP tracking efficiency, MPP tracking time, PV operating point fluctuation around MPP, controller input operating voltage range, battery type independence as well as temperature supply compensation.

Keywords: Solar System, MPPT charge controller, input operating voltage, Maximum power point tracking.

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Impact of Sn doping on the physical properties of ZnO sprayed thin films for use as solar cell electrodes

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Abstract

Due to their exceptional properties, zinc oxide (ZnO) thin films have demonstrated potential as transparent conducting oxides (TCOs), making them suitable for use in optoelectronics. To enhance the performance of this oxide, we have introduced tin (Sn) as a dopant in ZnO. We selected Sn for its conductivity and ability to easily replace zinc in the crystal lattice. In this work, pure and Sn-doped (0.5, 1, and 1.5 wt%) ZnO films deposited by spray pyrolysis were fully characterized. The effect of Sn doping on the structural, optical and electrical properties of ZnO has been investigated in order to improve the efficiency of solar cells. The X-ray diffraction analysis (XRD) determined that the thin films possess a polycrystalline structure, showing a preferential orientation along the (002) plane. Additionally, the Raman spectroscopy corroborated the presence of the wurtzite structure in all of the films. The increased Sn concentration improves the crystalline characteristics and increases crystallites size from 31.5 nm to 34 nm. The FESEM images reveal a granular composition of nanostructured spherical grains with increased density as a result of Sn doping. According to the AFM analysis, adding 1% Sn to ZnO led to a substantial decrease in roughness, going from 21.66 nm to 6.81 nm for pure ZnO films and 1% Sn-doped ZnO films, respectively. The optical analysis reveals that all thin films exhibit a high transparency, estimated at approximately 74%. Additionally, the direct optical gap of pure ZnO films increased from 3.25 to 3.29 eV with 1% Sn doping. The electrical properties of ZnO films are enhanced by the addition of Sn, achieving a low resistivity value of 3.18×10^{-2} Ω.cm and a high figure of merit (FOM) of 1.22×10^{-4} Ω^{-1} for the 1% Sn-ZnO thin film. These features make the 1% Sn-doped ZnO thin film a viable alternative for a transparent electrode in solar cells.

Keywords

Sn-doped ZnO, Spray pyrolysis, Optical gap, Resistivity, Figure of merit.

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Sol-gel synthesis of $Zn_{0.9-x}Co_{0.1}Al_2Cr_xO_4$ nanoparticles and investigation of their properties

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The Pure zinc aluminate ($ZnAl_2O_4$) samples and co-doped $ZnAl_2O_4$ with Chromium (Cr^{3+}) at varying ratios (2, 4, 6, 8, 10 mol%) alongside a constant Cobalt (Co^{2+}: 10 mol%) concentration were synthesized using the citrate sol-gel technique and subsequently annealed at 900°C for 3 hours. Various characterization methods were employed to examine the structural and optical properties, including powder X-ray diffraction (XRD), differential scanning calorimetry (DSC), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, and UV-visible spectroscopy. X-ray diffraction analysis indicated that all samples contained cubic, single-phase $ZnAl_2O_4$, devoid of impurity phases, and exhibited a nanometric crystallite size. The results were validated through Fourier transform infrared and Raman spectroscopy.

The photocatalytic study of various $ZnAl_2O_4$ samples demonstrated their effectiveness as photocatalysts and adsorbents for the degradation of methylene blue dye in aqueous solutions.

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$^{90-110}$Mo isotopes study within *Crancking Nilsson Strutinsky* model

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Abstract

The *Crancking Nilsson Strutinsky* (CNS) model is used to interpret the molybdenum isobar bands of A=90-110. The total energies are calculated and compared with the observed values. The most favorable configurations are asseigned and the deformation parameters (ε_2, γ) are determined to explore the shape evolution of these nuclei.

Keywords: isobar A=90-110, Crancking Nilsson Strutinsky, configurations, deformation parameters, triaxiality.

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Hydrogen Production from Thermochemical Cycle a Thermodynamic Study

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In this paper, a thorough study of a new hydrogen production cycle through Thermal water analysis using three chemical reactions based on copper chlorine is conducted. It is considered a new cycle.

This new configuration of the proposed hydrogen production cycle is modeled and analyzed comprehensively. This cycle has not been previously considered in the literature. The first configuration of this new cycle represents the cycle with a thermochemical character only (no electricity or electrolyser), this cycle can use solar energy or any thermal source, such as the heat released by the exhaust gases of the conveyance or gas turbines to be operational. Further transformations are adapted to the proposed CU-Cl cycle in order to overcome the problems encountered.

Various evaluations are achieved using several tools of thermodynamic and Thermo-chemistry modeling such as the endothermic or exothermic heat, enthalpy and entropy, besides the exergy destroyed. In the end, we get the efficiency of the last reaction of hydrogen produced approximately 88% which is a very positive result. This modeling is conducted by the energy simulation software EES.

Keywords: Hydrogen production; Water dissociate; Exergy and Energy analyses; thermochemical process; Environmental Sustainability.

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Path integral solution for the time-dependent Hamiltonian systems involving quadratic, inverse quadratic and $(1/\hat{x})\hat{p}+(1/\hat{x})\hat{p}$ terms

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Using the path integral method with space-time transformations, we obtain the exact solution for time-dependent Hamiltonian systems involving quadratic, inverse quadratic, and $(1/\hat{x})\hat{p}+(1/\hat{x})\hat{p}$ terms. The propagator is calculated, and the wave functions are derived.

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Non-Relativistic Spectrum of a Position-Dependent Mass Nonlinear Harmonic Oscillator

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Abstract

Position-dependent effective mass (PDEM) originates from the approximation of the effective mass of a many-body system in condensed matter physics. PDEM system theory has attracted a lot of attention due to the advent of sophisticated technologies for growing ultra-thin semiconductor structures, with very significant quantum effects. Many contributions to the fundamental understanding of the problem have been made from different perspectives. We will approach the solution of the Schrödinger equation for bound states by considering an interesting model proceeding by the generalized supersymmetry approach in quantum mechanics. In many areas of relativistic and nonrelativistic physics, the concept of supersymmetry is frequently used, and supersymmetric quantum mechanics (SUSYQM) has become a distinct academic discipline. In addition, the actual potentials meeting the shape invariance criterion in the SUSYQM paradigm are precisely soluble within the Schrödinger equation. In particular, we are interested in determining the limit states of a mass particle dependent on the position and subject to a unidimensional harmonic potential. The method used to obtain the solutions is based on the concepts of supersymmetric quantum mechanics and shape invariance. In order to illustrate the general formalism, a class of nonlinear oscillators has been considered. This class includes the particular example of a one-dimensional oscillator with different effective mass profiles as a function of position. The mass distribution is taken as $M(x)=((\beta^2)/(\beta^2-x^2))$ if $x>-\beta$ and the potential is considered as $V(x)=\frac{1}{2}Mx^2\omega^2$ where ω is a positive real constant. The spectrum and the corresponding wave functions are thus exactly obtained and special cases are discussed.

Keywords: Position-dependent mass; nonlinear harmonic oscillator, Schrödinger equation,

Supersymmetric quantum mechanics, shape invariance condition.

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Numerical investigation of forced convection heat transfer in cavity with obstacles using nanofluid T_iO_2/water

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Abstract: This study presents a numerical investigation of forced convection heat transfer in a cavity containing three rectangular obstacles positioned on the upper and lower walls, utilizing Titanium oxide T_iO_2/water nanofluid as the working fluid. The flow enters the cavity at a uniform temperature of 300 K, while the lower wall is maintained at a constant temperature of 350 K. The analysis covers a range of Reynolds numbers from 200 to 400 and explores different volume fractions of nanofluid, specifically 3% and 5%. The Nusselt number is calculated to assess the heat transfer performance within the cavity. Results indicate that the incorporation of T_iO_2 nanofluid significantly enhances the Nusselt number, demonstrating the positive influence of nanofluids on thermal performance in forced convection scenarios.

Keywords: Nanofluid, forced convection, Heat Transfer, T_iO_2/water, cavity with obstacles

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Impact of Quantum Error Suppression Techniques in Ground State Energy Estimation Using VQE

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Abstract

Variational Quantum Eigensolver (VQE) has emerged as a promising hybrid algorithm that utilize quantum and classical techniques to estimate the molecular ground state energies. Despite the noise generated by Near-Term devices pose a significant challenge for practical application we need the reduction in the noise levels of the expectation value estimated. Here, we perform VQE simulations on a molecular system using an IBM noise model simulator to study the impact of error suppression techniques. We implement Pauli twirling and dynamical decoupling sequences to mitigate noise effects and evaluate each technique's impact on error reduction. Our work highlight the performance of each method in improving the fidelity of energy estimates, providing valuable insights into optimizing error suppression techniques in quantum simulations for molecular systems.

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Metal-insulator electronic transition phenomenon in binary compounds under pressure and optical properties

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Abstract

The effect of pressure on the structural, elastic and electronic properties of the intermetallic compounds XAu (X=K, Rb and Cs) with a CsCl-type structure have been investigated using ab-initio calcul. The optical properties have been studied under normal pressure. We have carried out the plane-wave pseudopotential approach within the framework of the first-principle density functional theory (DFT) implemented within the VASP code. For the first time we have investigated the optical properties, mechanical and electronic properties under pressure of KAu (-3GPa), RbAu and CsAu (3GPa). The calculated band structures indicate that RbAu and CsAu are half-metallics at 0 GPa with indirect band gap (R→X) 0.3583 and 1.4274 eV respectively, whereas KAu compound is metallic. Furthermore, the phenomenon transition half-metal to metal in the RbAu and CsAu compounds is performed under moderate pressure (3GPa), while this transition of the KAu is obtained at about (-3GPa) with indirect energy gap (R→X) 1.33 eV. The most important elastic properties including the bulk modulus B, shear modulus G, Young's modulus E and Poisson's ratio ν of the cubic CsCl (*cP2*) type structure of XAu are determined under pressure by using the Voigt-Reuss-Hill (VRH) averaging scheme. The results show that the AuK intermetallic became mechanically unstable under (- 3GPa) pressure, but the RbAu and CsAu remained stable under (3GPa) pressure. Finally, the reflectivity spectrum shows that the reflectivity is high in the ultraviolet region up to 3 eV, for KAu, RbAu and CsAu.

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Nuclear shell model calculations in Zn isotopic chain on the neighbourhood of ^{56}Ni core

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Significant advances in experimental techniques and radioactive beams have allowed the exploration of more exotic nuclei and the explanation of isotopic sequences within the nuclear chart. These nuclei have long been a central topic in nuclear structure and dynamics. The information regarding the excitation energies of individual states and the nucleon-nucleon interaction that can be derived from each region of the nuclear chart provides a basis for testing the fundamental components of nuclear shell model calculations [1].

Furthermore, nuclei in the nickel region exist in shape coexistence in their nuclear structure. These coexistences refer to the ability of a nucleus to adopt different nuclear shape configurations at relatively close energies, which makes their theoretical and experimental study particularly interesting. This behaviour in other isotopes of the nuclear chart challenges our simplistic view of spherical nuclei. An improved comprehension of this phenomenon will contribute to a better understanding of the fundamental properties of nuclear matter [2].

The objective of this study is to examine the influence of the pairing gap energy effect within the context of the nuclear shell model. We are interested in the Zn isotopes surrounding the ^{56}Ni doubly magic core. We investigate some calculations of nuclear spectroscopic properties such as low-state excitation energies and gamma transition probabilities of even-even nuclei [3]. The calculations are performed in the framework of the nuclear shell model using the NuShellX@MSU [4] nuclear structure code. This study is based on the jj44pn valence space consisting of eight proton and neutron orbitals with recent experimental values of single-particle energies outside the ^{56}Ni core. Various effective interactions [5] have been adopted in the pn-formalism. This work aims to provide a detailed description of the nuclear structure and shape evolution of these isotopes. The obtained results showed a reasonable correlation with the available experimental data in the low-lying yrast and yrare states of these even nuclei.

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Particle in an infinite square well influenced by a Rosen-Morse potential

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In this work, we aim to analyze the behavior of a particle with mass m moving inside an infinite square well of finite width under the influence of an additional, general potential $U(x)$ using the path integral approach. The particle is then subjected to a potential defined by

$$V(x) = V(x) + U(x), \qquad (1)$$

where

$$V(x) = \begin{cases} 0 & 0 < x < 1 \\ \infty & \text{elsewhere,} \end{cases} \qquad (2)$$

and the Lagrangian of the system is given by

$$L(x, x, t) = \frac{m}{2}\dot{x}^2 - V(x) - U(x). \qquad (3)$$

We will construct the path integral for this system in phase space, where we will adopt the Dirac delta functional method [1]. An explicit calculation of the propagator will be obtained for two specific cases of the potential $U(x)$, namely the constant potential and the Rosen-Morse potential [2]. Both cases are transformed into the Pöschl-Teller potential [3], thereby reducing the problem under consideration to the Morse potentia. Finally, the energy levels and the wave functions for the bound states are derived.

Firstly, it should be noted that if x_f or x_i are outside the interval [0, 1], the propagator is zero, with $V(x)$ being infinite. However, if both x_f and x_i belong to [0, 1], the propagator is written in the phase space path integral form

$$K(x'', p'', t''; x', p', t') = \int Dx(t)\, Dp_x(t) exp\{(i/\hbar) \int_{t'}^{t''} dt\, [p_x \dot{x} - {p_x}^2/2m - V(x) - U(x)]\}. \qquad (4)$$

In order to deal with such a problem, we must bring the Hamiltonian into another form that permits a direct and explicit treatment of the path integral. For this purpose, we first make a point canonical transformation $(x, p_x) \rightarrow (q, p)$ defined by

$$x = f(q) = arg\, th(-cos(\pi q), \qquad q = (1/\pi) arccos(-th(x)),$$

$$p_x = (p/f\,'(q) = \pi^{-1} sin(\pi q)\, p. \qquad (5)$$

Finally, to give a conventional form to the propagator, we make the following temporal transformation $t \to s$

$$ds/dt = 1/f'^2(q). \qquad (6)$$

Therefore, the Green's function associated to the system is written as

$$G(q'', q'; E) = (g(q'')g(q'))^{1/4} \int_0^\infty ds \int Dq(s)\, Dp(s)$$

$$\times exp\{(i/\hbar) \int_{s'}^{s''} ds\, [p\dot{q} - p^2/2m - \frac{\pi^2}{sin^2(\pi q)} U(q)$$

$$+(\pi^2/8)(cos^2(\pi q) - 2 - 8E)/sin^2 \pi q]\}, \qquad (7)$$

where

$$g(q) = f'^2(\mathrm{q}) = \frac{\pi^2}{sin^2(\pi q)}, \quad q'' = \left(\frac{1}{\pi}\right) arccos(-thx_f) \; and \; g(q') = \left(\frac{1}{\pi}\right) arccos(-thx_i)$$

At this level, it is evident that we cannot perform explicit calculations due to the general form of the potential $U(q)$. Therefore, we must choose appropriate forms for this additional potential that allow us to enlarge the class of integrable systems which can be exactly solved using the delta functionals technique. For this purpose, let us consider a specific form for $U(q)$, namely the Rosen-Morse potential $U(x) = U_0 tanh^2(x) \to U(q) = U_0\, cos^2(\pi q)$. This potential reduces the studied problem to that of a particle inside the Pöschl-Teller potential hole of the $V \propto 1/sin^2(\pi q)$. Then, by leveraging the connection between the Pöschl-Teller potential and the inverse quadratic oscillator, we have exactly derived the bound state energies and the corresponding wave functions, which are successively given by :

$$E_n = \left(\frac{\hbar^2 \pi^2}{8m}\right)(2n+1)^2 \quad and \quad E_{U_0} = -\left(U_0 + \frac{1}{4}\right). \quad (8)$$

$$\Psi_n(x) = \sqrt{\frac{i}{\pi^2\left(U_0 - \frac{1}{8}\right)}} \frac{(-1)^{\frac{n}{2}} 2^{(\mathrm{n}+1)\Gamma^{\frac{1}{2}}}(-n)}{\sqrt{n!}\,\Gamma\left(-n+\frac{1}{2}\right)} \exp(-\frac{\lambda_e}{\hbar} x)$$

$$\times [\tanh(-x)]^{\mathrm{n}} F\left(-\frac{n}{2}, -\frac{n}{2}+\frac{1}{2}, -n\,; \frac{1}{tanh^2(x)}\right), \qquad (9)$$

where $\lambda_e = \frac{1}{2}\sqrt{m(2 + 8E + 8U_0)}$.

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Electrical Characterization of a Polycrystalline Silicon Solar Cell

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This study focuses on the modeling and analysis of the electrical characteristics of a polycrystalline silicon solar cell, a key technology in the field of renewable energy. Photovoltaic solar energy plays a crucial role in the energy transition, and optimizing solar cells is essential to maximize their efficiency.

Using MATLAB/SIMULINK software, three parametric models (L3P, L4P, and L5P) were developed to evaluate electrical performance through current-voltage (I-V) and power-voltage (P-V) curves. The study examines the influence of several critical parameters, such as series resistance, shunt resistance, the diode ideality factor, and saturation current, on the cell's performance.

The results reveal that the L4P model provides the best representation of the solar cell's electrical behavior, enabling efficient performance optimization. This research offers valuable insights for the development of more efficient photovoltaic cells, contributing to the advancement of solar technology and more effective use of solar energy in various contexts.

Keywords: Modeling, Characterization, Renewable Energy, Solar Cell, Photovoltaic.

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Effect of Mg concentration on the structural and optical properties of PVC/ZnO/Mg composite films used as photocatalysts for Orange II degradation

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Abstract

In this work, flexible photocatalysts based on PVC/ZnO/Mg composite films was fabricated using polyvinyl chloride as a polymer substrate. ZnO/Mg particles were successfully synthesized by coprecipitation method using a mixture of zinc nitrate and magnesium acetate. The effect of Mg-doping concentration (0 – 20 wt.%) on the physical properties of ZnO particles was studied. XRD patterns showed that all samples had a high degree of crystallinity in the hexagonal wurtzite structure of ZnO, with the crystallite size ranging from 19 to 21 nm. UV-Vis spectrophotometer revealed that Mg doping increased the bandgap energy of ZnO from 3.12 to 3.18 eV, while the bandgap energy of PVC decreased from 4.29 to 2.93 eV due to adding the ZnO/ Mg fillers. Hall effect measurements revealed that all samples had n type conductivity. Finally, to confirm the effect Mg doping concentration on the photocatalytic activity of ZnO, the degradation of Orange II using PVC/ZnO/Mg photocatalyts was studied. In particular, PVC/ZnO/Mg-10% sample exhibits a high photocatalytic activity compared to other samples. This result indicates that the polymer as a dielectric material has a promising future as a flexible substrate worth exploiting.

Key words: Coprecipitation, Photocatalyst, ZnO, Polymer, Mg, Orange II.

1. Introduction

In recent years, semiconductor-based metal oxides have become a focal point of research in the field of photocatalysis due to their good physical and chemical properties. Many metal oxide semiconductors have been used in the photocatalytic process, most notably titanium oxide and zinc oxide **[1, 2]**. In this work, we chose to use zinc oxide because it has been widely utilized as an effective and environmentally friendly catalyst due to its good chemical stability, high electron mobility, non-toxicity, and ease of preparation. Enhancing the efficiency of zinc oxide through doping is one of our objectives in this work. The second objective is more related to the economic aspect. Using magnesium-doped zinc oxide as a powder makes it impossible to recover and reuse multiple times. Therefore, we chose to use a Polyvinyl Chloride (PVC) as polymer matrix to preserve and recover the catalyst material for multiple uses. Our choice of PVC was due to the reliance of factories on plastic in sewage channels.

2. Material and methods

ZnO/Mg powders were synthetized by coprecipitation method, using zinc nitrate, magnesium acetate and distilled water. The mixture was stirred at 70 ° C for 2 h. Then, the powders were dried at 100 °C for 12 h and annealed at 550 °C for 2 h. PVC/ZnO/Mg composite films were synthetized by casting method, using polyvinyl chloride.

3. Results and discussion

From Fig.1(a), all the peaks are indexed to the hexagonal wurtzite structure of ZnO with high intensity. Fig.1(b, c) show that the powders have agranular appearance with good films forming. Fig.2(a, b) show the absorbance and transmittance spectra of the samples, the films are highly transparent. The Tauc plot was used to obtain the bandgap energy of ZnO. From Fig.2(c), Hall effect measurements revealed that all samples had n type conductivity. Fig.2(d) confirm the effect of Mg doping concentration on the photocatalytic activity of PVC/ZnO/Mg films, for decomposing the Orange II.



Fig.1. (a): X-ray diffraction patterns of ZnO/Mg particles (0-20 wt.%). **(b):** External appearance of powders and the disks of composite films. **(c):** Optical micrographs of composite films.

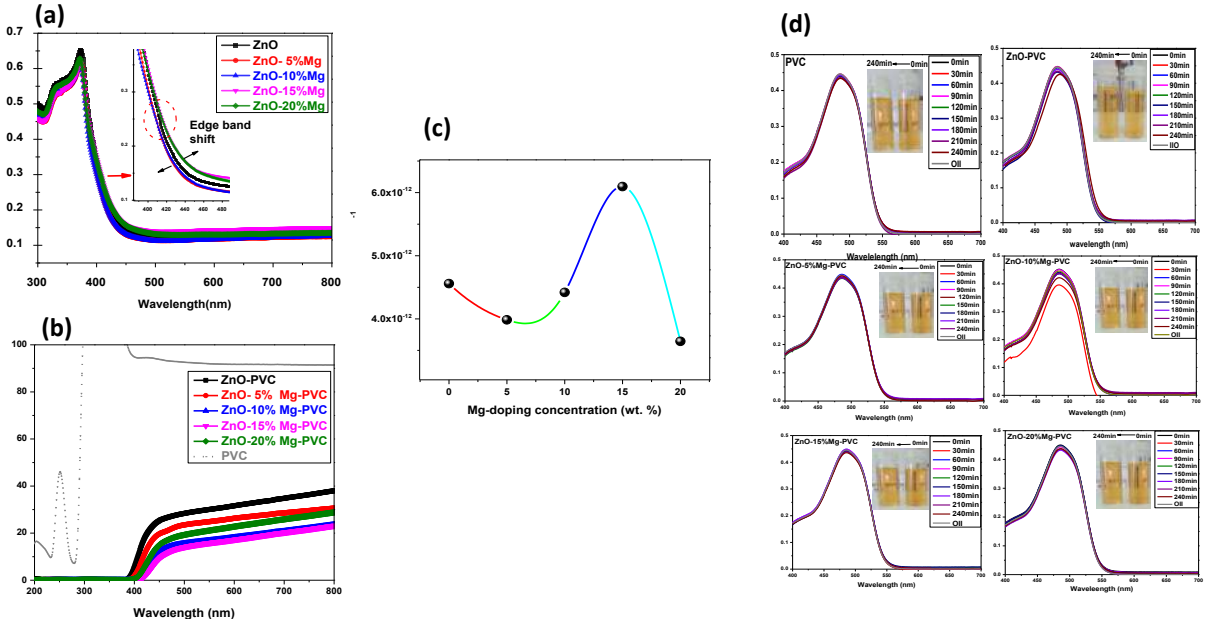


Fig.2. (a): Absorbance spectra of ZnO/Mg particles (0 – 20 wt. %). **(b):** Transmittance spectra of ZnO/Mg/PVC composite films. **(c):** Mg Effect on the conductivity of films. **(d):** Temporal variations of OII absorbance, degraded by using ZnO/Mg/PVC composite films, under UV irradiation.

4. Conclusion

From these results, PVC/ZnO/Mg-10% films exhibits a high photocatalytic activity compared to other samples. This result indicates that the polymer has a promising future as a flexible substrate.

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Occurrence of Bubble Structures in Z=8-20 Nuclei Using Skyrme-HF Plus BCS Approach

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Abstract

In this study, we systematically investigated the occurrence of bubble structures in light nuclei with proton numbers ranging from Z=8 to Z=20. Our approach combined the Skyrme-Hartree-Fock (HF) method with the BCS approximation to explore nuclear structures in isotopic chains including $^{12-26}$O, $^{16-34}$Ne, $^{20-40}$Mg, $^{22-44}$Si, $^{28-48}$S, $^{30-54}$Ar, and $^{36-60}$Ca. By analyzing nucleon densities and related structural properties, we identified several promising candidates for bubble nuclei, a class of nuclei characterized by a reduced central nucleon density.
Eighteen different Skyrme interactions were employed, including LNS, Sk3, KDE, NRAPR, Skz1, Skz2, Skz3, Skz4, Skm*, Skm1, SLy6, SLy7, SLy8, SLy9, SLy10, KDE0, SKRA, and KDE0v1, as proposed by Margueron et al. [2] and Grasso et al. [3]. These interactions allowed for a comprehensive study of the nuclear characteristics that promote bubble formation [2, 3], offering deeper insights into the exotic phenomena occurring in light nuclear systems [5, 4].
Our findings contribute to the broader understanding of nuclear matter and bubble structures in atomic nuclei, with implications for both nuclear theory and experimental detection of bubble candidates.

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Experimental Detection and Theoretical Analysis of Bubble Nuclei via Shell Model Calculations

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Abstract

Bubble nuclei represent an exotic class of nuclear systems characterized by a central region of reduced nucleon density, which poses a fascinating challenge to our understanding of nuclear structure [1, 2]. In this work, we explore the properties of medium-sized bubble nuclei using shell model calculations. We extend the classical harmonic oscillator mean field by introducing new potential models, including the spherical well, Morse potential, double Woods-Saxon potential, and a modified Morse potential. These models allow for a deeper investigation into the form factor, charge density distribution, and single-particle energy levels of bubble nuclei.

Our analysis reveals the presence of new magic numbers, 18 and 32, in medium nuclei, with significant effects on the occupation of low angular momentum states due to the bubble structure. Additionally, we propose a criterion for identifying bubble nuclei experimentally through the analysis of form factor ratios, offering a potential tool for experimental nuclear physicists. Specific candidates for bubble nuclei, such as 28Ne, 30Mg, 52Ca, 54Ti, and 56Cr, are suggested based on our results.

This study advances our understanding of bubble nuclei and opens new avenues for experimental verification in medium and exotic nuclear systems [3, 4, 5].

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Empirical calculation of total K-to-L shell vacancy transfer probabilities using interpolation methods for some elements

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In this study, we introduce a novel method for estimating total vacancy transfer probabilities $\eta_{KL}(T)$ based on well-established experimental data. We compiled a comprehensive experimental database of $\eta_{KL}(T)$ values for elements in the atomic range $57 \leq Z \leq 71$ and calculated the weighted average values $\eta_{KL}(T)$ for each element [1].

This work is particularly significant due to its wide-ranging applications in fields such as physical chemistry, material science, and medical research, where accurate vacancy transfer probabilities play a crucial role in modeling atomic behavior and radiation interactions.

A plot was generated to illustrate the relationship between the weighted averages and atomic number Z. Utilizing the analytical function $(\eta_{KL}(T))_W = a_0 + \sum_{i=1}^{N} a_i Z^i$, we interpolated new values for these elements. A thorough comparative analysis was conducted, comparing our results with theoretical predictions and other experimental or fitted $\eta_{KL}(T)$ values found in the literature. Our findings generally show a high level of agreement with previous studies, further validating the robustness of our approach.

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The η pseudohermitian Hamiltonian in the presence of minimal length concept

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Abstract:
New commutation relations in deformed space lead to a non hermitian Hamiltonian of harmonic oscillator model . The energy spectrum is found to be entirely real in the presence of the concept of minimal length. So, the □: pseudohermiticity □□□□□□ □ □□ of the physical system is discussed and important results are obtained. Especially the construction of □ and □ observables.

Keywords : deformed space, minimal length, hermiticity, pseudohermiticity.

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Modulating the Optoelectronic Properties of Ta_2O_5 through Controlled Incorporation of Silver Nanoparticles

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Abstract

Tantalum pentoxide (Ta_2O_5), a wide-bandgap semiconductor with exceptional dielectric properties, faces limitations in visible-light-driven applications due to its inherent absorption characteristics. This study investigates a novel approach to enhance the photoactivity of Ta_2O_5 by incorporating silver nanoparticles (AgNPs) at a 1% w/w loading via silver (Ag^+) fixation onto the Ta_2O_5 surface followed by controlled calcination. We systematically varied the calcination temperature (300, 500 and 700°C) to elucidate its influence on the resulting nanocomposite's structural and optical properties. X-ray diffraction (XRD) analysis revealed the presence of crystalline β-Ta_2O_5 and the formation of silver oxide (AgO) phases, with crystallite sizes influenced by the calcination temperature. Scanning electron microscopy (SEM) provided insights into the morphology and distribution of the AgNPs within the Ta_2O_5 matrix. Furthermore, UV-Vis spectroscopy demonstrated a notable shift in the absorption edge of the nanocomposites towards the visible light region, suggesting enhanced light harvesting capabilities. A detailed correlation between the observed optical modifications and calcination conditions will be discussed, highlighting the potential of these Ag/Ta_2O_5 nanocomposites for enhanced photocatalytic and optoelectronic applications. This work contributes to the ongoing effort to develop efficient visible-light-driven photocatalysts by strategically manipulating the interaction between plasmonic nanoparticles and wide-bandgap semiconductors.

Key words: Wide bandgap semiconductor, Ag /Ta_2O_5 nanocomposites, Metal – Oxide Interactions, Optical features.

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Infrared behvior of next-to-leading order energy of ultrasoft transverse photon in hot SQED

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Abstract
In recent years, there has been steadily increasing activity aimed at analyzing the phase structure of Quantum Chromodynamics (QCD), the quantum field theory of strong interactions. A detailed understanding of the properties of the deconfined phase of QCD, the so-called Quark-Gluon Plasma, is important in several areas of Physics. Examples are the evolution of the early Universe [1], heavy ion collisions at RHIC (Brookhaven) and LHC (CERN) [2]. A major problem that spurred progress in the late 1980's was the apparent gauge dependence of the one-loop order quasiparticle dispersion relations, most notably the gluon damping rate. The problem was resolved in [3]. It turns out that in order to calculate consistently at high temperature, we have to use an effective perturbation that sums the so-called hard thermal loops (HTL) into dressed propagators and vertices [3], [4]. The first next-to-leading order physical quantity that has been determined in the framework of the HTL program is the zero-momentum transverse gluon damping rate [5]. It was shown to be finite and positive. Subsequent studies of the behavior of the gluon and quark damping rates in the imaginary-time formalism have indicated that there are difficulties in the infrared sector [6-12], A similar observation has been done in the context of scalar electrodynamics [13]. To look further into the infrared behaviour, we propose to calculate the next-to-leading order dispersion relations for slow-moving Transverse Photons at high-temperature scalar quantum electrodynamics (Scalar QED), using the real time formalism (RTF) in physical representation. We derive the analytic expressions of hard thermal loop (HTL) contributions to propagators to determine the expressions of the effective propagators in RTF that contribute to the complete next-to leading order contribution of retarded Transverse photons self-energy. The Transverse retarded photons self-energy is related to the next-to-leading order energy.
Keywords: Hard thermal loop, Hot Scalar QED, NLO Computations, Soft Transverse photons energy, Infrared divergences

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Beyond SM Physics and searches for SUSY at the LHC

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Abstract

We briefly review the Standard Model (SM) and the major evidences and main direction of physics beyond the SM (BSM). We introduce supersymmetry, as one of the well-motivated BSM. Basic introduction to Minimal Supersymmetric Standard Model (MSSM) is given. We analyze the thermal relic abundance of lightest neutralino, which is the Lightest Supersymmetric Particle (LSP) in the MSSM. We show that the combined Large Hadron Collider (LHC) and relic abundance constraints rule out most of the MSSM parameter space except a very narrow region. We also review non-minimal SUSY model, based on the gauge group $SU(3)_C \times SU(2)_L \times U(1)_Y \times U(1)_{B-L}$ (BLSSM), where an Inverse Seesaw mechanism of light neutrino mass generation is naturally implemented. The phenomenological implications of this type of model at the Large Hadron Collider (LHC) are analyzed.

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Resolving the $B \to D^{(*)}\tau\bar{\nu}_\tau$ decays anomalies in non-minimal SUSY model

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Abstract

We explain the recent combined experimental results from Belle, BaBar and LHCb of the ratios $R(D)$ and $R(D^*)$ provided by the Heavy Flavour Averaging (HFLAV) group. We show that $R(D)$ and $R(D^*)$ can be explained simultaneously in the B-L extension of the minimal supersymmetric Standard Model with inverse seesaw through the right-handed sneutrino contribution in the lepton penguin.

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Investigating Swift Heavy Ion Irradiation in SiO_2 Thin Films: A Combined TREKIS-3 and Inelastic Thermal Spike Approach

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Abstract

When a thin film material such as SiO_2 is bombarded by MeV-energy swift heavy ions (SHI), a significant portion of the deposited energy is transferred to the target atoms, primarily through inelastic electronic collisions. This process leads to intense excitation and ionization within the film, initiating a variety of damage mechanisms, ranging from the creation of point defects to surface sputtering[1], erosion, and even sublimation of the thin film material.

This study investigates the effects of SHI on SiO_2 thin films by combining the TREKIS-3 simulation code[2] with the inelastic thermal spike (i-TS) model. The i-TS model explains how the energy deposited by the ions is first transferred to the electronic system, resulting in localized electronic excitation. The energy is then transferred to the atomic lattice, leading to rapid heating and atomic displacements, which drive structural changes in the thin film. The TREKIS-3 code complements this by simulating ion-solid interactions, providing a detailed understanding of energy deposition and material response in thin films.

This combined approach offers valuable insights into the inelastic energy deposition mechanisms, which result in structural modifications such as defect formation, phase transitions, and surface damage specific to thin films. This methodology provides a comprehensive framework for predicting SHI-induced effects in SiO_2 thin films, making it highly applicable for use in microelectronics, photonics, and energy storage technologies. Furthermore, it has potential applications in radiation detection systems, such as silicon barrier detectors, and can be used to study the irradiation effects through sputtering mechanisms for surface modification and material analysis in thin films.

Keywords: swift heavy ions, SiO_2 thin films, TREKIS-3 code, inelastic thermal spike model, ion-solid interactions, ion irradiation defect.

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Effect of dipping time on the structural ,optical properties and ultraviolet photoresponse property of sol-gel dipcoated SnO_2 films

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In this work, pure tin oxide SnO2 thin films were prepared by Sol-gel dipcoating method on ordinary glass substrates heated to 5500 C, using as precursor (SnCl2 ,2 H20) dissolved in ethanol , we changed in this films dipping time (20s ,40s, 60s and 80s).

This films were characterized by X-ray diffraction, UV-visible spectroscopy, by SEM scanning electron microscopy and UV photoconductivity.

The XRD spectra exhibit a tetragonal rutile structure with a preferential directin along (110) with the grain size 3,2nm calculated by debye scherrer's formula, optical transmittance showed high transparency ,the value of the optical band gap energy is 4eV.at 2V applied voltage and at 40s as dipping time ,there is high photocurrent for the film.

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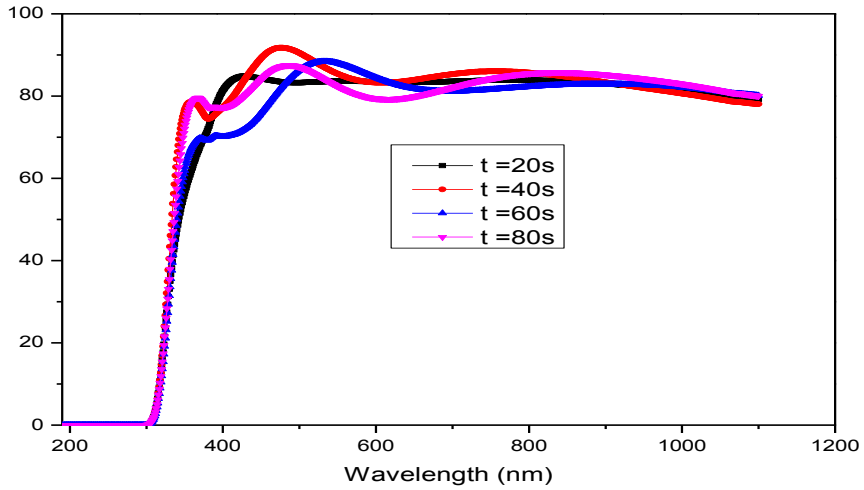


fig1

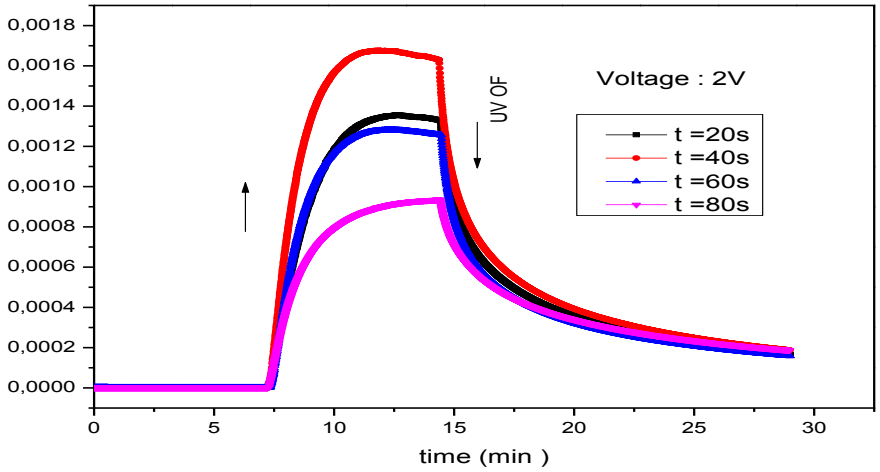


fig2

Table : The values of photocurrent, dark current and Ion and Ioff

Dipping time of the sample t (sec)	Photocurrent I_{on} (A)	Dark current I_{off}(A)	I_{on}/I_{off}
20	0.00136	$1{,}72.10^{-6}$	790,697
40	0.00168	$8{,}78.10^{-7}$	1913,439
60	0.00128	$1{,}13.10^{-6}$	1132,743
80	$9{,}35.\ 10^{-4}$	$8{,}53.10^{-7}$	1096,131

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A comparative study of the first instability appearance in forced and mixed convection in a vertical Taylor-Couette system subjected to a constant heat flux

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This work presents a comparative numerical study of the first Taylor instability in a Taylor-Couette system, composed of a rotating adiabatic inner cylinder and a fixed outer cylinder subjected to a constant flux. The generated heat is transferred to a flow of distilled water in the annular space.

The study aims to deepen understanding of instability mechanisms by identifying the critical Reynolds numbers for both cases: forced and mixed convection, with the goal of optimizing the ideal one for industrial heat systems that involve rotational flows.

The model of the conservation equations (mass, momentum, and energy) and its associated boundary conditions is numerically solved using the finite volume method with a second-order spatiotemporal discretization.

The results obtained show that natural convection delays the appearance of the first instability by generating an upward axial flow, transforming the first Taylor instability (TVF) into a spiral instability (SPI), thus modifying the behaviour of the forced convection regime.

Key words: *Spiral instability, Finite Volume method, Taylor Vortex Flow, Constant flux, Mixed convection.*

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computational study of vibrational frequencies of C,p-methoxyphenyl-N-phenyl nitrone

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Abstract

The density functional theory (DFT) with the three-parameter hybrid functional (B3) for the exchange part and the Lee–Yang– Parr (LYP) correlation function calculations has been carried out in the present investigation [1], using density functional method (B3LYP) 6-31G(dp) with Gaussian 09 program package. From that the optimized structure and the vibrational frequencies were calculated.

The first task for the computational work was to determine the optimized geometry of C,p-methoxyphenyl-N-phenyl nitrone compound. The calculations converged to an optimized geometry which corresponds to an energy minimum. The vibrational frequencies were evaluated using density functional theory (DFT) with the standard B3LYP/6-31G(d,p) basis. The Raman and IR spectrums are characterized by a series of bands in the 250–3250 cm-1 spectral range. In-plane C– H stretching bands were observed in the 1024.7-1337.8 cm^{-1} range [2]. The asymmetric and symmetric C–H stretching bands appear in the 3250–3000 cm^{-1} range [3] and C–C ring stretches in aromatic compounds appear in the 1600–1400 cm^{-1} region [4].

The assignments of the calculated normal modes have been made on the basis of the corresponding PEDs. The PEDs are calculated from vibrational frequencies calculated by quantum chemistry, using the VEDA 4 program [5].



Figure: Optimized geometry of C,p-methoxyphenyl-N-phenyl nitrone

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Numerical Simulation of Heat Transfer in Biological Tissues for the Treatment of Arrhythmias

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Abstract:

Thermal ablation is a medical technique used to treat cardiac arrhythmias by selectively destroying the tissues responsible for electrical abnormalities. This study proposes numerical modeling and simulation of heat transfer in biological tissues to optimize the ablation procedure.

We employ the Pennes bio-thermal model to describe the heat diffusion generated by different energy sources, such as radiofrequency (RF) or high-intensity focused ultrasound (HIFU). Partial differential equations (PDEs) are solved numerically to simulate the temperature evolution within cardiac tissues. The model also accounts for blood perfusion effects, which act as a cooling mechanism, ensuring a realistic thermal process simulation.

We studied the impact of different power levels on the temperature evolution over time. The simulations reveal that higher power levels lead to faster temperature increases, reaching necrosis thresholds within a few seconds.

This approach provides a scientific foundation for improving the precision and safety of thermal ablation procedures. The numerical results obtained offer insights into integrating these models into clinical practice, particularly through patient-specific simulations based on medical imaging data.

Keywords: Numerical simulation, Thermal ablation, Thermal modeling, Radiofrequency, HIFU, Arrhythmia, Optimization.

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An experimental assessment of a novel eco-friendly insulating material reinforced with date palm fibers.

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Abstract:

This investigation aims to assess the impact of integrating sustainable and biosourced materials into brickwork as heat-insulating materials, with the goal of improving thermal comfort in buildings. A practical solution for reducing energy consumption is the development of environmentally favorable composites as insulating materials in buildings. In light of the aforementioned factors, this study introduces a novel biocomposite material that incorporates natural fibers, such as date palm fibers, clay, and sand. Additionally the study also examines the effects of inclusion date palm fibers to bricks, including their ability to insulate against heat, save energy, and absorb water. This new biocomposite material is meant to be used in building construction, where the size of the fibers was 0.4 mm. The analyzed specimens contained a proportion of date palm fiber that varied from 0% to 5%. The resistance to heat, thermal conductivity, and absorption of water of the specimens were experimentally determined. The results suggest that increasing the weight of the date palm fiber results in a decrease in thermal conductivity and increase resistance to heat, as well as an increase in water absorption. The thermophysical properties of the composite material are considerably improved by the inclusion of date palm fiber, which in turn increases the insulating capacity of the brick.

Keywords: Sustainable, Date palm fibers, Biocomposite, Natural fibers, Thermal conductivity

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Nuclear di-clustering in the framework of U(14) and U(14)⊗U(14) models

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The atomic nucleus is a system of A interacting nucleons. It may happen that such a system shows a more exotic configuration where groups of nucleons form clusters. Such feature affects the nuclear structure.

Many light nuclei can be considered as a system of clusters [1] due to the high binding energy of the alpha particle. However, in heavy nuclei it is usually assumed that the ground state is mainly a zero-cluster state. With increasing excitation energy one-cluster states appear. Such states have already been described using the algebra U(4)⊗U(4) by Daley and Iachello [2]; later two extensions have been introduced [3][4].

As it has been predicted by Ikeda, di-cluster states occur at higher excitation energies; their description needs a new mathematical frameworks. In the present work we present a model based on the U(14) algebra and its extension to the more complex U(14)⊗U(14) algebra. The model is able to unify zero, one and two-cluster states, either in IBM- I or IBM-II. In the first version we introduce three s bosons, two p bosons and a d boson. The number is doubled in the second version due to the distinction between proton and neutron bosons.

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Assessment of a Passive Solar Distiller's Performance in Arid Conditions: A Case Study at URERMS Adrar, Algeria

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This project presents the design, construction, and results of a simple passive solar distiller installed at the Research Unit for Renewable Energies in Saharan Region URERMS in Adrar, Algeria, with the primary objective of evaluating its performance under summer and winter climatic conditions.

The solar distiller was designed to be both simple and efficient, leveraging principles of solar energy conversion to produce distilled water from brackish water. It consists of a solar collection surface, a condensation system, and a storage reservoir, all constructed using locally available materials to ensure durability and practicality.

Tests were conducted over a period of six months, encompassing both summer months characterized by intense sunlight and high temperatures, and winter months with reduced solar brightness. Data collected included daily production of distilled water, solar conversion efficiency, and seasonal performance variations.

Results demonstrated that the solar distiller could generate a significant amount of distilled water even during winter months, although production was higher in summer due to increased solar intensity. Evaluation of solar conversion efficiency, calculated as the ratio of incident solar energy to distilled water produced, was crucial in assessing overall system performance.

This study underscores the importance of developing local and sustainable solutions to meet water needs in arid regions such as Adrar. The solar distiller exhibited the capability to operate effectively throughout the year, despite pronounced seasonal variations, highlighting its potential to contribute significantly to sustainable water resource management in challenging environments.

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Compact Object in modified gravity

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Abstract

Compact objects, such as black holes, neutron stars, and white dwarfs, are dense remnants of stellar evolution, with their structures governed by strong gravitational fields and quantum effects. A key feature of their dynamics is the emission of gravitational waves, particularly through quasi-normal modes (QNMs)—oscillations characterized by complex frequencies. QNMs arise as perturbations in the spacetime around compact objects and provide insights into their intrinsic properties like mass, spin, and charge. These modes represent damped oscillations, where the real part of the frequency corresponds to the oscillation rate and the imaginary part to the decay rate. Studying QNMs is crucial for gravitational wave astronomy, as their detection offers a powerful tool to test General Relativity and probe the nature of compact objects, potentially revealing exotic physics such as the existence of non-Kerr black holes or modifications of gravity.

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Effect of plant extract concentration and precursor volume ratios on the formation of copper oxides nanoparticles and their Antibacterial Activity.

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An ecological synthesis method of copper oxides nanoparticles (CuO-NPs) has been successfully performed using a leaf extract of Pelargonium graveolens "Géranium roast". The study focused on the influence of several parameters such as extract concentration and the volume ratios between extract and precursor solutions, on the morphological, structural and physical properties of CuO-NPs.

In order to examine the functionality of these nanoparticles, the tests of antibacterial activity were performed on gram – positive and gram- negative bacterial strains. In a typical synthesis, 150 ml of 0.025M $CuSO_4.5H_2O$ solution was mixed with 50ml of different plant leaf extract concentration (0.025g/ml, 0.05g/ml, 0.15g/ml, 0.1g/ml 0.2g/ml and 0.5g/ml) prepared by hydro distillation procedure, with 3:1 as a volume ratio, precursor solution was slowly dropwise with constant magnetic stirring.

To study the different physical properties of the as synthesised nanopowders, several characterization techniques were used. The crystalline properties and phase purity was characterized by X-ray diffraction. Scanning electron microscopy was used to analyse the morphologies of as – prepared samples. The elemental composition of CuO-NPs was analysed by energy dispersive X-ray, FTIR and Raman spectroscopy. The gap energy of the materials was estimated by Tauc -plot method from UV-Vis measurement.

XRD analysis confirms that all biosynthesized copper oxide NPs have a monoclinic crystalline structure of cupric oxide CuO. However, for the very low concentration of precursor, copper hydroxide $Cu(OH)_2$ appear as a metastable phase. The average crystallite sizes estimated by the Scherrer formula vary between (9.92 and 16.3 nm). The morphological properties of CuO-NPs nanoparticles revealed by SEM characterization shows a like-flakes and nano-rice forms. EDX data showed that the product consisted of very pure CuO NPs. The Raman study exhibits the existence of Ag and 2Bg characteristic vibration modes in the CuO-NPs phase. The transformation of $Cu(OH)_2$ to CuO oxide nanoparticles was confirmed by FT-IR spectroscopy. The FT-IR spectra show the formation of copper oxides after annealing states. The band gap has been found at around 1.23 to 1.29 eV.

Further, antimicrobial activity was observed in samples prepared at a 0.1 g/ml extract concentration. The observed values of antibacterial activity were 17.5 ± 0.01 mm for Gram-negative (Escherichia coli) and 15 ± 0.02 mm for Gram-positive (Staphylococcus aureus) bacterial strains.

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First principle calculations of The Structural and optical properties of the Cubic perovskite RbSrBr3

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Halide inorganic perovskites have emerged as a promising material for optoelectronic applications due to their exceptional properties.Their large molar absorption coefficient, narrow photoluminescence bandwidth, high carrier mobility, and low recombination rate make them ideal candidates for a variety of devices, including solar cells, light-emitting diodes (LEDs), photodetectors, photocatalysts, and anti-counterfeiting technologies [1].

In this study, we investigated the structural and optical properties of the rubidium-based cubic halide perovskite, RbSrBr3. Employing the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) based on the Density Functional Theory (DFT) intergated in the WIEN2K code, we calculated the lattice parameter and optical parameters such as the dielectric constant, refractive index, reflectivity, absorption, and optical conductivity.

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The influence of mechanosynthesis on the structural and thermal properties of nanocrystalline alloys

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Keywords: Mechanical alloying (MA), Nanocrystalline materials, $Ni_{80}Co_{20}$ alloy, X-ray diffraction (XRD), differential scanning calorimeter (DSC).

ABSTRACT

In recent years, the development of nanostructured materials has experienced incredible results due to their potential applications in various technological fields (electronics, catalysis, magnetic data storage, etc.). When the grain size is reduced to the nanometre scale, the chemical, physical and mechanical properties of nanomaterials become excellent and better than those of bulk materials [1]. Nanostructured NiCo alloys are known by their potential applications in biomedical engineering due to their excellent mechanical properties. Nanocrystalline alloys can be obtained by various processes, one of which is mechanical alloying (MA), a method of processing a wide variety of nanomaterials in the solid state. This process leads to stress deformations that create many defects such as vacancies, dislocations, stacking faults and grain boundaries [2].

The $Ni_{80}Co_{20}$ alloy was prepared by mechanical milling of pure Co and pure Ni powders in a Retsch EMAX high performance ball mill. The powder was placed in two jars with steel balls and sealed in an aerobic environment at room temperature. In order to avoid overheating inside the jars, the synthesis was carried out by milling followed by rest cycles. XRD measurements were used to analyse the phase evolution, structural and microscopic parameters of the powder mixture as a function of milling time. The XRD patterns were taken in the range of 2Θ [30-130] ° with a step size of 0.02°. The Thermal measurements were carried out using a differential scanning calorimeter (DSC) in the temperature range [25-550] °C in an argon atmosphere with a heating rate of 10 K/min.

X-ray spectra of $Ni_{80}Co_{20}$ alloy powders were taken at different milling times (0 h, 3 h, 12 h, 24 h) (figure 1).It was observed that with increasing milling time the intensity of the peaks decreases and their diffraction peaks broaden, which can be explained by the decrease in crystal size, L, from 98.5 to 12.3 nm, accompanied by a significant increase in microstrain from 0.0163% to 0.421% in 24 h for the fcc-Ni (Co) phase. The lattice parameter increases during the milling time from 0.3524 nm to 0.3536 nm due to the fact that Co-fcc has a slightly larger radius than Ni-fcc, so that Co gradually dissolves into the Ni network leading to an increase in the lattice parameter, which can also be attributed to particle expansion associated with the increase in dislocation density [3].

The dislocation density is one of the critical structural parameters affecting the microstructure of the sample. It increases throughout the MA process between 0 and 24 hours from $2.3*10^{13}$ $/m^2$ to $4.7*10^{15}$ $/m^2$ due to the severe plastic deformation generated during the milling process, corresponding to the continuous decrease in crystal size during the milling process. [4].

The DSC thermograms of the $Ni_{80}Co_{20}$ alloy in Figure 2 revealed endothermic reactions at the beginning of heating between [50-80] °C and exothermic reactions in the temperature range [300-400] °C, associated with the relief of internal stresses accumulated during the casting process. [4].

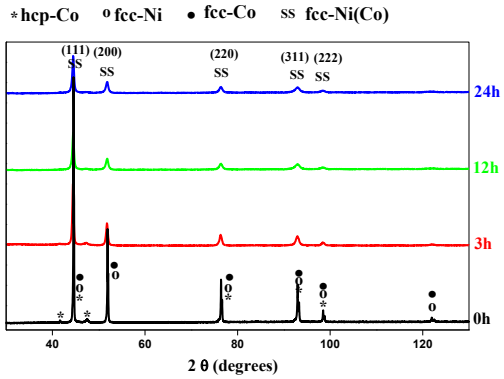


Figure 1: Evolution of XRD patterns of $Ni_{80}Co_{20}$ powders as function of milling time

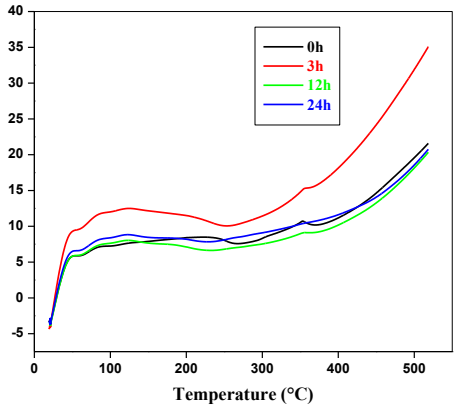


Figure 2: DSC thermograms of $Ni_{80}Co_{20}$ milled mixtures as function of milling time

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Effect of calcination temperature on the structural and magnetic properties of Cobalt Ferrite ($CoFe_2O_4$) nanoparticles Synthesized by Auto-Combustion

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Cobalt ferrite ($CoFe_2O_4$) nanoparticles exhibit unique magnetic, structural, and optical properties, rendering them suitable for applications in magnetic data storage, catalysis, and spintronics. This investigation examines the influence of calcination temperatures (500°C, 700°C, and 800°C) on the structural and magnetic properties of $CoFe_2O_4$ nanoparticles synthesized via the auto-combustion method. X-ray diffraction (XRD) analysis confirmed a cubic spinel structure across all samples, with enhanced crystallinity at higher temperatures. The grain size increased from 4.18 nm at 500°C to 12.43 nm at 800°C, attributed to augmented atomic diffusion. More pronounced diffraction peaks at elevated temperatures indicated a more defined crystal structure[1]. Fourier-transform infrared spectroscopy (FTIR) revealed significant absorption bands at 550 cm^{-1} and 410 cm^{-1}, associated with metal-oxygen bonds, confirming the successful formation of the $CoFe_2O_4$ phase[2]. Magnetic properties were significantly influenced by calcination temperature. Saturation magnetization (Ms) increased substantially from 7.08 emu/g at 500°C to 79.77 emu/g at 800°C, correlated with improved crystallinity and larger particle size, which enhanced magnetic domain alignment. Conversely, coercivity (Hc) decreased from 1236.3 G at 500°C to 1117 G at 800°C, indicating a transition to softer magnetic behaviour[3]. This investigation elucidates the critical role of calcination temperature in determining the structural, optical, and magnetic properties of $CoFe_2O_4$ nanoparticles, suggesting that optimizing these parameters is essential for enhancing their performance in magnetic and optoelectronic applications.

Keywords: Cobalt ferrite, structural properties, calcination, magnetic properties,

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Derivation of a Modified KdV Equation and Analysis of Solitons and Double Layers in a Quark-Gluon Plasma Using the Reductive Perturbation Method

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In previous work, it was shown that KdV solitons can exist in QCD [1] under two specific conditions: first, the gluon field must have a dynamic mass, and second, there must be second-order derivative terms in the energy density [2] . These conditions have led to the derivation of the modified Korteweg-de Vries (mKdV) equation in this study, which admits solitons and double layers as solutions.

Solitons and double layers were analyzed within the context of a quark-gluon plasma. Using the reductive perturbation method [3], a modified KdV equation was derived. The existence domains of solitary waves and double layers were established, and their parametric dependencies were determined. This theory is more general, as it explains the behavior of nonlinear periodic waves, as well as compressive and rarefactive mKdV solitons and double layers in a quark-gluon plasma.

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Investigation of Photocatalytic Electrochemical Performance through Green Synthesis Using Lavender Extract

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The integration of plant extracts into electrochemical applications offers a novel and environmentally sustainable approach [1], utilizing their inherent biochemical properties to enhance the performance and stability of electrochemical devices.

In this study, lavender leaf extract was employed to synthesize ZnO nanostructures, which were subsequently deposited onto copper substrates using the spray pyrolysis technique. The synthesized ZnO nanostructures were thoroughly characterized using electrochemical methods [2].

Electrochemical impedance spectroscopy (EIS) revealed the catalytic capabilities of the ZnO nanostructures. Moreover, current-voltage (J-V) measurements demonstrated an increased current density under illumination, indicating notable photocatalytic activity in the ZnO nanostructures [3].

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Search for a signal of Z' decaying to a top quark and a vector-like top quark within LRSM at LHC

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Abstract

Standard model (SM) of particle physics is an extremely successful theory from theoretical and experimental perspectives. Even though, it still incomplete theory where it doesn't give an answer for several problems.

One of the most attractive extensions beyond the SM is the left-right symmetric model (LRSM) [1, 2, 3, 4, 5]. The model has been developed mainly to accommodate parity violation in weak interaction and offer an explanation for neutrino masses through see-saw mechanism [6]. The gauge structure of LRSM allow the existence of extra charged W' and neutral Z' gauge bosons. Research for extra gauge bosons was the main interest of many experiments at the LHC, since a wide range of theoretical models predicts them [7, 8, 9, 10, 11, 12, 13, 14].

An other problem which the SM suffer from is the quadratic divergence in Higgs mass. However, it could be expalined by adding a new exotice kind of particles called vector-like quarks (VLQs) [15, 16, 17, 18], where the quantum corrections from the top chiral quark and the top vector-like quark will annihilate each other [19]. Moreover, these new heavy states can be produced in different manners at LHC and are consequently an important goal of many searches for new physics [20, 21, 22].

Search for heavy gauge bosons decay to heavy T and B VLQs and one of the third generation quarks has been investigated recently at a center-of-mass energy of 13 TeV by the CMS collaboration [23, 24]. Thus, we gives an alternative model for the LRSM contains one generation of VLQs. Both chiral parts of the VLQs are associated to the fundamental representation of an extra gauge factor $SU(2)_V$. Consequently, their masses can be generated through direct mass terms in Lagrangian. Moreover, results from atomic parity violation experiments and LEP collider puts strong constraints on the mixing of the VLQs to the first and second generations of the ordinary quarks [25]. Thus, we consider that they mix just with the third generation.

In this paper we are interested by the decay of Z' to a t quark and a heavy vector-like top quark partner T. T itself will decay through th and tZ channels by branching fractions 20/80%. The calculation is done by making use of narrow width (NW) and Breit-Wigner (BW) approximations. We demonstrate that the NW approximation is valid for wide range of parameter space, whether for Z' or T, thus we can make a comparison with the experiment conducted by CMS collaboration in [24]. The results indicate that the Z' in our model still unconstrained by the experiments, thus achieving more precision in future experiments is required for constraning our model.

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Daytime variation of OI 557.7 nm emission in the Earth's upper atmosphere: Model simulations and Observations

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Abstract

In this study, an excited metastable $O(1S)$ model was developed to analyze the 557.7 nm dayglow emission in the Earth's upper atmosphere using the EUVAC solar flux model, the 1D Boltzmann kinetic equation, and the fluid transport equations. The study involves the use of computational numerical models because many processes such as electron impact, ion-neutral-metastable chemistry and ambipolar diffusion are occurring simultaneously and contribute to the overall objective. The volume emission rate of the OI line at 557.7 nm shows a marked variation with altitude, solar zenith angle, and solar activity, represented by the $F10.7$ solar index. The current modeled results are compared with observations from the remote sensing instrument WINDII. The results show an improved agreement with these measurements.

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Impact of Nanofluid Physical Properties on the Efficiency of Additively Manufactured Heat Sink

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Abstract

The impact of nanofluid properties on the thermal performance of a 3D-printed heat sink was studied numerically. The heat sink, with a bottom wall measuring 40 x 40 mm², features mini-channels equipped with aluminum fins and is wrapped in an acrylonitrile-butadiene-styrene (ABS) copolymer for insulation. Two types of nanofluids with distinct physical properties were used: Al_2O_3-water and Cu-water. A constant heat source of 350,000 W/m² was applied under the lower wall of the heat sink, while the flow rate and temperature of the nanofluid at the inlet were kept constant.
The equations governing physical phenomena were solved using the finite volume method. The results are presented in the form of streamlines, isotherms, and temperature diagrams.
The study showed that the properties of nanofluids significantly influence the temperature of the heat source as well as the flow rate in the heat sink. Moreover, the ABS copolymer used for insulation has improved the thermal transfer between the walls of the mini-channels with fins and the heat transfer fluid, thereby enhancing the overall thermal performance of the device.

Key Words: nanofluid, micro-fin heat sink, additive manufacturing, acrylonitrile-butadiene-styrene (ABS)

Geometric shape of the heat sink



Figure 1: 3D printed heat sink.

Some results

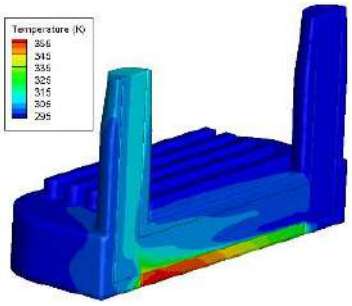


Figure 2: Temperature distribution (Cu-water nanofluid)

Table 1. Thermophysical properties of the nanoparticles

	ρ (kg/m^3)	Cp $(J/kg.K)$	k (W/mK)	β $(1/K)$
Cu nanoparticles [1]	8933	385	401	1.67×10^{-5}
Al_2O_3 nanoparticles [1]	3970	765	40	0.85×10^{-5}

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Photoelectrochemical properties of TiO_2 Nanofibers sensitized by polyol-made QDs: Comparative study

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Abstract

Nanoparticles synthesized by polyol process with well-defined crystallinity were assembled into TiO_2 nanofibers (NFs) by chemical bath deposition with an aim to improve their photoelectrochemical properties. The photoelectrochemical (PEC) properties of the resulting nanostructures were measured, using a homemade electrochemical cell illuminated with a standard Xenon lamp, and compared to those of bare TiO_2 NFs and also to ZnS-TiO_2 and CdS-TiO_2 studied in the previous works. A net enhancement of the photocurrent was observed on CdS-TiO_2 photoanode, suggesting a low carrier recombination rate and a higher efficiency of the PEC device for solar water splitting, as the induced photocurrent is related to the electrons needed to reduce H^+ ions into H_2 at the cathode electrode (Pt wire).

Keywords

QDs@TiO_2 NFs photoanodes , Photoelectrochemical, comparative study

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INVESTIGATING THE ROLE OF VAN DER WAALS interactions in the electronic properties of encapsulated semiconducting zigzag CARBON NANOTUBE by a carbon-based linear chain.

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As an exciting new field in advanced materials, van der Waals (vdW) nanomaterials, have drawn a particular attention due to their interesting features and potential uses. For the 1D nanostructures, carbon nanotubes (CNT) can be considered by geniusly exploiting the hollow space inside the carbon nanotubes for the incorporation of selected molecules and consequently encouraging interactions between the host and the invited components. Indeed, encapsulating carbon linear chains within CNTs has been viewed as a focal point of recent research by the means of non covalent functionalization process since the role of the corresponding vdW interactions in these systems is crucial for the determination of the structural parameters and the electronic properties of the combined structures.

This study investigates the encapsulation of a single polyyne chain within the zigzag CNT (8,0), (both of the sub-structures are exhibiting semiconductor behaviors before the encapsulation), by dealing with different vdW functionals for modelling the interaction between the two components. The resulted system polyyne@CNT(8,0) provides new structural parameters and electronic band structure properties. We especially look forward the charge transfer between the two components in order to investigate the metallization effects as can be impacted on the invited carbon-based linear chain. This is studied in the context of the phase transition from the semiconducting polyyne to the metallic cumulene by examining the variation of the bond-length alternation (BLA) pertinent value before and after the encapsulation.

All the calculations are done with the GGA PBE pseudopotentials for the set of { C09, BH, DRSLL, LMKLL, VV } vdW functionals as implemented in the SIESTA software package code.

Keywords : Van Der Waals interactions, non covalent functionalization, encapsulation, zigzag CNT, carbon-based linear chain

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Hydroxyapatite forming ability of dicalcium silicate prepared from local raw materials

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In this study, Ca_2SiO_4 powders were synthesized using solid state reaction. The starting powders were sintered at 1050 °C for 2 h. Moreover, the in vitro bioactivity of β- Ca_2SiO_4 was investigated by soaking the powders in simulated body fluid (SBF) for 15 days to analyze the growth of hydroxyapatite (HA) on the surface of these powders.

The synthesized powders were characterized by scanning electron microscopy (SEM, Fourier transform infrared (FTIR), and Inductively Coupled Plasma- Optical Emission Spectroscopy (ICP-OES) analysis.

The simulated body fluid results showed that β- Ca_2SiO_4 powders had a good bioactivity to induce hydraxyapatite formation on their surface The results obtained showed that (HCA) can be formed on the surface of β- Ca_2SiO_4 soaked in SBF solution, and a continuous layer of dense deposits of HCA covered the surface of β- Ca_2SiO_4 powders after 15 days of soaking in SBF solution.

Finally, the results obtained suggest that β- Ca_2SiO_4 ceramics are promising candidates for bone regeneration.

Keywords: Bioceramics, In vitro tests, Simulated body fluid.

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Synthesis and Characterization of PEG-capped CuO-ZnO nanomaterials

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Metal oxides nanoparticles have gained considerable attention due to their unique physical and chemical properties making them highly suitable for applications in areas such as photo-catalysis, sensing and energy storage [1–2]. Among these, cupric oxide (CuO) nanoparticles are particularly interesting for their semiconductor behavior, ease of synthesis and wide range of applications, including antibacterial activity and photo-detection [3]. In an effort to further enhance the structural and optical properties of CuO, researchers have explored the introduction of other nanoparticles like zinc oxide (ZnO) and the use of capping agents such as polyethylene glycol (PEG) to stabilize and improve nanoparticles performance [1,4].

This study focuses on the synthesis and characterization of pure CuO nanoparticles, chemically precipitated CuO-ZnO nanoparticles and PEG-capped CuO-ZnO nanocrystals. PEG serves as a capping or stabilizing agent to prevent agglomeration and to enhance the stability of the nanoparticles. The synthesized nanoparticles were systematically analyzed for their structural and optical properties using techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR) and UV-visible spectroscopy (UV-Vis).

XRD analysis confirmed the presence of a monoclinic CuO phase (Tenorite) in all samples, while the CuO-ZnO and PEG-capped CuO-ZnO nanoparticles displayed additional peaks corresponding to the hexagonal wurtzite ZnO phase, notably a peak at a position of $2\theta = 36.6°$. The average crystallite sizes ranged from 13 to 16 nm for CuO and from 20 to 21 nm for ZnO, indicating effective crystallite formation and stabilization. FT-IR spectra validated the presence of characteristic Cu-O and Zn-O bonds, confirming the successful synthesis of CuO-ZnO nanocomposites and the effect of the PEG capping agent. The optical properties of these nanomaterials were further examined through UV-vis reflectance studies leading to a band gap of approximately 1.19 eV for the CuO nanoparticles.

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Numerical calculation of photovoltaic parameters CuO solar cells with SCAPS-1D

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ABSTRACT

The results presented in this paper discuss the effectiveness of thin film CuO solar cells. Using the solar cell capacitance simulator (SCAPS), an alternative structure of p-CuO/CdS/n-TiO2 has been suggested. The primary goal of this analysis is to enhance the efficiency of the device using cost-effective materials compared to previous generations. To achieve this, a 350 nm p-CuO layer was introduced. Different thicknesses of the p-CuO absorber layer, ranging from 350 nm to 550 mm, were tested. Our results indicate that increasing the thickness of the absorber layer leads to improved performance of the new CuO solar cells.This work involved using different temperature ranges (300K - 400K). It was determined that the optimal configuration should comprise a window layer (TiO2), a buffer layer (CdS), and an absorber layer (CuO) with respective thicknesses of 35nm, 150nm, and 550nm. Solar cells featuring these specifications achieved a conversion efficiency of 17.38% when tested under the AM 1.5 spectrum and 1000w/m2 illumination.

Keywords:SCAPS-1D, Thin films, solar cell, copper oxide

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Physical properties and magnetoresistance of La-based perovskite structure

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Abstract:

The physical properties of the $La_{1-x}Ca_xMnO_3$ phase compound have been investigated, focusing on the magnetoresistance phenomenon (MR) studied by electrical transport measurements [1-3]. These materials find extensive technological applications in magnetic sensors, photonic and optoelectronic devices, computer hard drive reader, logic devices.

In the aim to test the effect of doping by Y in this phase, ceramic samples of nominal composition of $La_{0.55-x}Y_xBi_{0.15}Ca_{0.3}MnO_3$(x= 0 and 0.2) are elaborated and characterized. An analysis at room temperature of X-ray diffraction data using the Rietveld refinement method showed all samples crystallized in the orthorhombic phase with Pnma space group, and all samples are of high purity. Scanning electron microscopy (SEM) analysis reveals that the doping by Y causes a significant change in the microstructure of the sample. The temperatures of magneto-resistivity curves are registered from room temperature under a magnetic field up to 5 Tesla and showed that the undoped sample present a metal-insulator transition (I-M) at a temperature TP ≈ 135, 83 K. Some physical parameters are extracted and their evolution with magnetic field are presented and discussed. The highest obtained MR value is about 91.81% at 5 Tesla.

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Analysis of the geometry effect on airflow behavior in a prototype of a Small New Vortex Tower

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The current work highlights the impact of dynamic thermal-hydraulic parameters, such as velocity, pressure, temperature, and turbulence kinetic energy, on the flow behavior inside a small-scale novel vortex with different geometry coupled with nuclear reactor's secondary circuit. The nuclear power plant cooling system and the realized Small-scale Novel Vortex Tower are linked to minimize the quantity of cooling water utilized from rivers or the sea. The density difference effect, which is the primary factor governing the vortex power, transforms the thermal energy of the heated air from a natural hot source into kinetic energy, which is then transformed into mechanical energy by means of turbines and converted into electrical power.

The idea is based on using the chimney effect to remove unused heat from the reactor's cooling tower, which allows the air kinetic energy to rise at the exit. Therefore, in order to recover as much energy as possible to meet our demands, it is crucial to identify the optimal place for thermal hydraulic property enhancement.

A three-dimensional numerical analysis using CFD code was carried out to simulate the dynamic and thermal airflow. The simulation results of the air flow parameters such as air velocity, temperature and pressure at different position along TV prototype are provided. The numerical model is validated by comparing the new velocity results of the Novel Vortex Tower Prototype with cylindrical chimney and the different new conception designs. For this last, the numerical preliminary results shown that the novel vortex tower model could generate an artificial vortex and upward airflow utilizing a heat source with a maximum air velocity of 4.81 m/s in the exit of the convergence chamber.

Keywords: Vortex tower, CFD, Artificial vortex generation; Modeling and simulation.

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Modeling and Simulation of a leakage in a counter flow heat exchanger using RELAP5 code

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Heat exchangers are extensively used in a wide range of applications, including production processes, transformation and energy utilization in the industry. A heat exchanger is a device designed to transfer heat from a hot fluid to a cold fluid without the two fluids coming into contact. The heat exchanger is usually connected to other thermal equipment and during operation; unexpected variations in operating conditions, such as variations in inlet flow rate or temperature can occur. These transient conditions can affect the overall system behaviour and the installation safety, potentially leading to significant economic losses. Therefore, knowledge of the heat exchangers thermal response is necessary either for process control, or to determine their impact on the various plant components. For this reason, the transient behavior of heat exchangers has been a subject of interest and study in industry and research, with various analytical and numerical methods employed to explore this topic.

This work presents a modeling and simulation of a leakage in the internal wall of a horizontal counter flow heat exchanger with concentric tubes using the Relap5/Mod3.2 system code, in order to predict the transient behavior of the heat exchanger following this incident. A heat exchanger model was developed and validated using steady and transient regime experimental data, and good agreement was obtained. To model the break, a Trip-Valve component 180 was employed, as shown in Fig. 2. Both qualitative and quantitative evaluations of the results were conducted by examining the water flow through the heat exchanger during transient conditions. The theoretical results are illustrated through graphs depicting the evolution of inlet and outlet temperatures, as well as flow rates of each fluid (Fig. 3).

The main simulation results demonstrate the ability of the Relap5/Mod3.2 code to track the time-dependent evolution of the heat exchanger's thermal-hydraulic parameters. In addition, the leak has a significant effect on the main heat exchanger parameters, leading to a disturbance of flow and heat transfer conditions, as shown by the fluid response along the heat exchanger.

Mots clés : Heat exchanger; Modeling and simulation; Relap5/Mod3.2, Steady-state, Leakage.

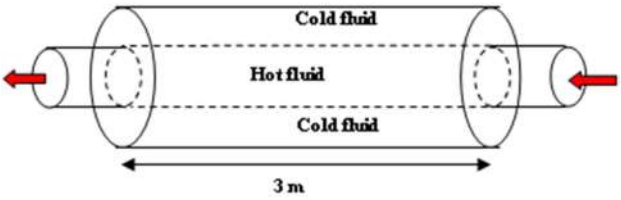


Figure 1. Heat exchanger with two concentric tubes.

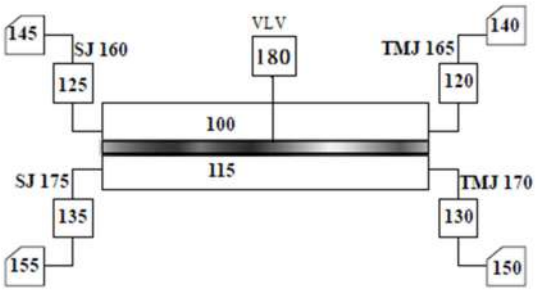


Figure 2. Heat exchanger nodalization diagram.

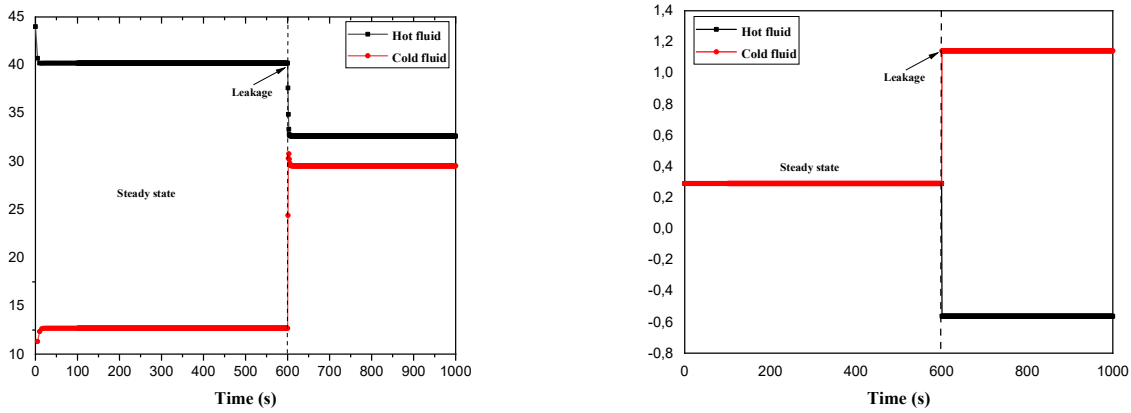


Figure 3. Temperature and mass flow rate variation during the leakage.

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Effect of Irradiation on the thermal stability of the PMMA

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Abstract

The main objective of this work is to study the effect of gamma γ irradiation on polymethyl methacrylate (PMMA). We will particularly focus on the variation in MASS and thermal stability and other key parameters following exposure to Gamma irradiation at a dose rate equal to 22 Gy/min and different absorbed doses. By exploring these aspects, our goal is to decipher the molecular and structural mechanisms responsible for the observed changes, while identifying the practical implications of these modifications for specific applications of PMMA in environments exposed to high irradiation levels.

To study the degradation and thermal stability of the PMMA film before and after radiation, the Thermogravmetric Analysis (TGA) technique was used. The analysis of some samples of irradiated PMMA by thermogravimetry (ATG) shows that gamma radiation does not influence mass losses, and the samples begin to degrade at different temperatures. Degradation is rapid then it becomes stable for doses 150kGy and 500kG, hence the use of the material at temperatures above 200°C could induce a breakage of certain chemical bonds in the main chain of the material.

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Application of copper oxide thin films for photocatalytic degradation methylene blue

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Spray pyrolysis technique was used to prepare copper oxide thin films by a low-cost method. We deposited pure thin films by changing the deposition time (5, 10, 15 and 20 min) using copper acetate as the source material dissolved in distilled water at a concentration of (0.1M). XRD spectrum confirm the formation of copper oxide in his two forms; cuprite Cu2O of cubic structure and tenorite CuO of monoclinic structure. The UV visible spectrum exhibit non-transparent films (12%) as a maximum transmittance for 5 min of sprayed. The optical gap is varying between 1.85 eV and 2.78 eV indicates the formation of tenorite phase instead of the cuprite phase. The vibration modes of cuprite structure were appearing around 636 cm-1 . The degradation rate of MB is found about 20% for 300 min of exposition to UV irradiation for the samples sprayed 5 min although the degradation rate for the samples sprayed 20 min is found around 3%

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The Passage Of Spacetime

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As a rule of thumb, one cannot ask about existence without addressing the issue of spacetime, just like it is impossible to understand the physical phenomenon without defining a clear concept of spacetime. As known, there is a noticeable advance in the history of physics that is highly related to the changes of the spacetime concept. Therefore, in this research, a new look at spacetime has been given, so that space and time becomes one thing in terms of their characteristics, as a change in time requires a change in space, and this is called Spacetime passage, which provides the necessary energy for objects to preserve their masses, properties, and existence. This may give a glimpse into the origin of the relationship $E=mc^2$. The spacetime tackled here is the spacetime of rest for particles, not the spacetime of motion. The spacetime in which the mass behaves as a clock of this spacetime, and in a scale where quantum effect takes place, so that the quantum phenomenon becomes conditional on studying the formation of matter. Thus, a relation between quantum state and the passage of spacetime has been done. In this way, the absolute and relative have been linked in quantum mechanics, and to gain further insight into the quantum phenomenon, the particle quantum jump and the essence of the wave-particle duality have been touched upon.

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Investigating the effect of the number of quark flavors on the behavior of some response functions for the thermal QCD deconfining phase transition

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In the framework of the study of the thermal Deconfinement Phase Transition (DPT) in a finite volume, within the bag model [1,2], we study in the present work the influence of the number of quark flavors on some response functions well characterizing the mixed hadronic matter-Quark Gluon Plasma (QGP) system at the transition. For this purpose, we consider two system cases: a 2*f* system meaning "two quark flavors system" containing u and d quarks in the QGP, and a 3*f* system containing u, d and s quarks in the QGP. In both cases, the hadronic matter is supposed to contain the lightest hadrons which are pions. We calculate the partition function of the QGP with the color-singletness requirement, using the projection method [3,4]. We calculate then an adequate order parameter for the occurring DPT, $\langle h \rangle$, defined within a phenomenological coexistence model [5-7], as well as the three first thermal derivatives of $\langle h \rangle$. The integral expressions of the studied quantities are then calculated numerically, and the graphs illustrating their variations with temperature, for various volumes are obtained. For the two system cases, we notice that the effective transition temperature in small volumes, shifted from the true one in the thermodynamic limit, can be defined at the value $\langle h \rangle$=0.5, meaning that both hadronic and QGP states contribute with equal probability to the total system. Similarly, it can be defined at the minimum of the first derivative representing the thermal susceptibility, at vanishing second derivative and at the maximum of the third derivative. Also, the width of the transition region over which the transition is rounded off can be defined as the gap in temperature between the extrema of the second derivative. The main result is that the transition temperature is lowered when considering three quark flavors in the QGP phase.

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computational approach to solve specific types of complex systems through discovering their exact structures

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In this research, we provide a unified computational model that describes the general structure of traveling wave solutions obtained by applying the functional component method for nonlinear long wave equations, which is based on a set of computational transformations and theorems using Mathematica software. This model can be used to solve a variety of complex problems as well as current instances of complex systems with dynamic applications.

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Silica-Supported $CoFe_2O_4$ nanoparticles as magnetically separable photocatalysts for ethyl violet degradation

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Abstract:

This work explores the synthesis and characterization of $CoFe_2O_4/SiO_2$ nanocomposite as effective photocatalysts for the degradation of ethyl violet, aiming to establish their potential in environmental applications. The nanocomposite was synthesized using wet chemical method followed by calcination at 700°C, leading to the formation of $CoFe_2O_4$ spinel nanoparticles, as confirmed by XRD. The unique morphology observed through TEM comprising both elongated (11 x 9 nm²) and spherical (9 nm) shapes provide a high surface area-to-volume ratio, which is crucial for enhancing the interaction between the catalyst surface and the pollutant molecules.

Optical studies revealed a broad absorption band between 240-430 nm with a maximum at 350 nm, corresponding to a band gap of 2.7 eV, which is within the ideal range for UV_A light absorption. This band gap allows efficient generation of electron-hole pairs, which are key to driving the photocatalytic degradation reactions.

The magnetic properties of the $CoFe_2O_4$ nanoparticles, characterized by superparamagnetic behavior, a high saturation magnetization (71 emu g^{-1}), and a coercive field of 295 Oe, facilitate the easy separation of the catalyst from aqueous solutions using an external magnetic field.

The BET surface area measurement (13 m^2 g^{-1}) highlights the catalyst's capacity to provide ample reactive sites for pollutant interaction, while maintaining sufficient porosity for mass transport during the degradation process.

Photocatalytic tests showed that $CoFe_2O_4$ nanoparticles achieved a remarkable photodegradation efficiency of 93 % within 60 minutes under UV_A irradiation. The kinetics followed a pseudo-first-order reaction with a rate constant of 0.033 min^{-1}, indicating rapid degradation of ethyl violet. These combined structural, optical, and magnetic properties not only explain the high photocatalytic activity of $CoFe_2O_4$ nanoparticles but also highlight their potential for large-scale

environmental remediation. The magnetic separability, in particular, adds a significant advantage, making the reuse of the catalyst in continuous processes more feasible.

Keywords: $CoFe_2O_4$ nanoparticles, superparamagnetic, photocatalytic efficiency, ethyl violet, wastewater treatment.

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Preparation and characterization of Li-doped ZnO thin films by sol–gel method

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In thus study Zinc oxide (ZnO) thin films have been prepared by sol gel technique using zinc acetate dihydrate dissolved in methanol, ethanol and deionized water [1] Undoped and Li doped ZnO thin films were deposited on a glass substrate. The films were prepared at 3 mol. % and 5mol. % of Li doped ZnO at 500°C annealing [2] In order to investigate the effect of Li doping on ZnO thin films properties on the crystallinity and morphological properties of ZnO films were assessed by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM) and XRD patterns of the films showed the hexagonal wurtzite type polycrystalline structure [3]

Also the samples were tested as UV photocatalyst for MB degradation, Firstly, diffraction patterns showed a hexagonal structure, for pure ZnO and 3%La_ZnO layers, and at 5 at.% the preferential orientation changes, and crystallite sizes range from 11nm to 18 nm. The FESEM study depicted that the uniformly distributed grains for all samples. The methanol sample showed greater grains for 5%Mg doped ZnO thin film [4]

The UV–visible analysis of the prepared layers shows high transparency (65–80%) in the visible range, with a constant optical gap of 3.36 eV.

The photo catalysis has gained significant research at tension because of their potential application in environmental conservation such as air and water purification, hazardous waste treatment together with energy production via green technology, [5]ZnO can decontaminate water by removing different types of dyes, including methylene blue (MB), (MO), rhodamine B, and different sorts of bacteria[6-7].

The photocatalytic activities of the coatings were tested via methylene blue degradation under UV light in an aqueous solution.exhibit superior photocatalytic activity under UV irradiation, showed the highest methylene blue photodegradation, reaching about 90% after 150 min of UV irradiation compared to a pure ZnO thin film for the same time.In terms of methyl blue degradation, the 5% Li doped ZnO thin films had a better degradation of 90%.

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Investigation of Sn doping effects on the properties of copper oxide thin films deposited by the spin coating method

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This work aims to investigate the effects of Sn doping on the optical properties of zinc oxide (ZnO) thin films deposited on glass substrates by sol–gel spin coating process and annealed in air for 2h at 500°C. The optical characteristics of prepared films were examined by UV–VIS spectrophotometer. UV–Visible spectrum exhibits a high transmittance for all the prepared films with a strong increasing versus photon energy in the visible range from 300 - 400 nm. The highest transmittance was observed for 1 wt % of Sn doping. The band gap value decreased slightly with increasing the Sn doping, higher and lower values were determined as 3.33 eV for 3 wt % and 3.19 eV for pure ZnO respectively. Urbach energy values increase with increasing Sn doping. The results show a strong ability of Sn doping to improve the properties of ZnO thin films, proving their suitability for several optoelectronic applications as conductive oxides and transparent electrodes.

Keywords: Sol-gel, spin-coating, ZnO thin films, Sn doping, optical properties.

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Top quark p_t distribution in the t-channel of single top quark production at hadron colliders within the non-commutative standard model

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Abstract

We present a phenomenological prediction concerning the transverse momentum distribution arising from the production of t-channel a single top quark at the Large Hadron Collider (LHC) within the framework of the non-commutative standard model (NCSM). Similar to the Standard Model, when we perform the calculations at leading order for both the NCG parameter Θ and the strong nuclear coupling α_S, we find that the transverse momentum distribution in the NCSM suffers from divergences at low p_t^{top}, which we eliminate through resummation. We observe in our analysis that the effects of non-commutative geometry are most pronounced in the middle of the distribution and diminish for very large p_t^{top}. In the low p_t^{top} region, the nature of the effects cannot be determined due to divergences in that region. Based on previous works, we expect that this region is not affected by corrections; therefore, we provide a direct matching technique that enables us to obtain results valid even at low p_t^{top} values, as achieved using standard model parton showers like `Pythia 8`.

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Constraints on the Noncommutativity Parameter

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The noncommutative space-time theories have been studied extensively; while the motivation for this kind of space-time with noncommuting coordinates is mainly theoretical. The first idea that space coordinates may not commute was suggested by Heisenberg **[1]** and formalized by Snyder **[2]** and there has been an immense amount of challenge devoted to the subject of noncommutative space-time, it has been realized that noncommutative geometry plays a distinguished role in the formulation of string theory **[3, 4]** and M-theory **[5]**. The noncommutative field theory **[6]** has been constructed by introducing the Moyal product in the space of ordinary functions, and by defining field theory in quantum phase space. Equivalence between these two approaches has been clarified in Ref.**[7]**. Phenomenological aspects of space-time noncommutativity have been analyzed using a noncommutative extension of the standard model **[8]**.

Physics in noncommutative space-time and phase spaces has been extensively investigated in literature. In this work, we explore the consequences of time-space noncommutativity in some scattering processes, focusing on the Moyal plane with just time-space noncommutativity; we compare our presentation with the different presentations of the noncommutativity parameter $\theta_{\mu\nu}$, and we discuss that the scale of the space-time coordinates noncommutativity if it could be larger than the Planck length.

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Effect of thickness on ankle-foot orthosis resistance using numerical modelling

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Abstract

Various 3D printing technologies allow for easy, fast, efficient, and cost-effective production of ankle-foot orthoses (AFO) using polymer materials, making orthotics a prominent area of research. This study aims to predict the resistance of AFO to 3D printing using the polymer resin of the DLP 3D printer through thickness variation based on numerical modelling of AFO that simulates foot flexion under real conditions. This study focuses on improving AFO manufacturing with this advanced printing technology by predicting critical regions and analysing stress concentration on polymer AFOs, while evaluating the relationship between stiffness and mechanical properties of the material using the finite element analysis method.

Keywords: Numerical Modelling, Ankle-Foot Orthosis, 3D-Printing, Polymer.

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L'effet du nombre de Rayleigh sur la convection naturelle dans une cavité carrée remplie d'un nanofluide

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Ce travail traite la convection naturelle dans une cavité carrée remplie d'un nanofluide newtonien (nanoparticule « **Ag** » **et** fluide « **Eau** ») qui est incompressible, stationnaire, bidimensionnel et laminaire. Les parois haute et base étant considérées à une température chaude T_{ch}et les parois gauche et droite sont maintenu à une température froide T_{fr}.

Pour une fraction volumique ($0 \leq \phi \leq 0.2$), en voir l'effet du nombre de Rayleigh (varie entre 10^3 et 10^5) sur les champs thermique et les champs de vitesse et sur Le nombre de Nusselt moyen Nu_m, qui caractérise le transfert de chaleur. Les équations sont résolues par la méthode des volumes finis, en utilisant un schéma de "Power-Low" pour discrétiser les termes convectifs et non linéaires de l'équation d'énergie. Les résultats numériques obtenus par implémentation du code de calcul Fortran montrent que le taux de transfert de chaleur augmente avec l'augmentation du nombre de Rayleigh, et l'effet des nanofluides sur la convection naturelle présente des valeurs de Rayleigh beaucoup plus élevées.

Mots clés : Transfert de chaleur, la convection naturelle, nanofluides, nombre de Rayleigh, cavité carrée.

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New Semi-Empirical Formula for (n, t) Reaction Cross Sections

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A semi-empirical formula is proposed to calculate excitation function for the (n, t) nuclear reaction at 14.6 MeV. This semi-empirical systematic contains free parameters fixed by experimental data, we use pre-equilibrium exciton model to describe tritium emission in nuclear reactions induced with rapid neutrons. To verify the quality of the proposed formula, we compare the obtained cross-section with measured ones. We found that calculated (n, t) excitation function is close to the experimental data and the proposed systematic better describes tritium emission for even-even nuclei target.

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Search new physics beyond the standard model in e^+e^- colliders

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In this work; we present a novel extension of the standard model, wherein we explore various scattering phenomena in $e^-\ e^+$colliders, such as: Bhabha scattering, Moller scattering, leptons production, production of particles within the framework of the non-commutative standard model (NCSM) we employ Seiberg- Witten (SW) maps with the first-order consideration of the (NC) parameter $\theta^{\mu\nu}$. this model is founded on the noncommutativity of the space-time: $[X^\mu, X^\nu] = i\theta^{\mu\nu}$. Our focus lies on investigating the angular distribution of the cross-section $\frac{d\sigma}{d\Omega}$,building upon prior research, to scrutinize the impact of noncommutativity at the TeV scale and to contrast it with results obtained from the standard model (SM). This endeavor aims to assess the validity of the NCSM at high energy scales. The results obtained indicate deviations in the angular distribution, highlighting geometric effects at the level of jet production.

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Optimizing Hydrogen Absorption Rates Through Reactor Geometry and PCM Integration

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This research explores the influence of reactor geometry and phase change material (PCM) integration on hydrogen absorption rates in LaNi5 metal hydride reactors. Using computational fluid dynamics (CFD) simulations, three reactor configurations with distinct geometric structures and PCM arrangements were evaluated. The study's objective was to improve heat and mass transfer efficiency, thereby optimizing hydrogen absorption kinetics.

The results showed that Design 3, integrating PCM more effectively, achieved the fastest hydrogen absorption rates. In this design, hydrogen concentration reached saturation within 1.5 hours, compared to over 4 hours in Design 1. Furthermore, the PCM melting behavior was analyzed, and Design 2 demonstrated superior energy storage capabilities, achieving a 90% liquid fraction within 3 hours.

Natural convection and heat transfer were examined using the Nusselt number and heat transfer coefficients, with Design 3 showing significant improvements. The study found that effective reactor geometry combined with optimal PCM placement enhances the system's thermal management, allowing for faster hydrogen absorption and improved energy storage efficiency.

These findings provide valuable insights into the design and optimization of hydrogen storage systems, particularly in applications requiring high-performance thermal management, such as electric vehicles and renewable energy systems.

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A V_2 gauge leptoquark for the $R_{D^{(*)}}$ anomalies

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Abstract: We present a possible ultraviolet (UV) completion of the vector leptoquark representation $V_2 = (\bar{\mathbf{3}}, \mathbf{2}, 5/6)$ as an attempt to accommodate the experimental hints of deviations in semileptonic decays of B mesons in charged currents. Tree-level analyses of simplified models have recently shown that a TeV scale vector leptoquark V_2 is an interesting candidate to explain the $R_{D^{(*)}}$ anomalies. We take the next step forward and embed it into a non-abelian gauge theory where ordinary color, isospin and hypercharge are partially unified with an $SU(5)$ gauge symmetry in order to examine loop-induced effects as there are severe constraints in $\Delta F = 2$ processes.

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Stuady of the effect of Bi doping on the structural properties and optical of Co3O4

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Abstract

This research examines the effects of Bismuth-doped Co3O4 thin films on their structural, morphological, optical, and electrical properties at varying concentrations of Bismuth (0, 2, 4, 6, 8, and 10 wt%). Bismuth-doped Co3O4 thin films were fabricated on glass substrates utilising a custom spray pyrolysis apparatus at 400 °C. Structural studies indicated that these films possess a spinel cubic structure preferentially orientated along the (111) direction. The crystallite size diminishes With doping . The optical transmittance of films improved to 63% for 4 wt% Bi-doped Co3O4 films and subsequently dropped. The maximum conductivity value of 6.656(Ω cm)-1 was achieved for the 8 wt. % Bi-doped Co3O4 films.

Keywords: Co3O4, doping, Bismuth, Spray pyrolysis.

1 Introduction

Transition metal oxide materials (TMO) have attracted the attention of many researchers as a promising material for technological application due to their electronic, optical, and technological properties, such as their flexible elemental composition, good ferroelectric properties, adjustable band gaps and catalytic stability, and their abundance of soil and less toxicity. Among the transition metal oxide, we find cobalt oxide, the latter of which has attracted the attention of researchers in various applications, and we find it in three stages: Coo, Co2O3 and Co3O4. Among them, we find Coo rocksalt and ordinary spinel Co3O4 have a stable crystalline structure; Coo quickly oxidises in the open air and leads to the formation of Co3O4.

Therefore, Co3O4 is the most stable. Its thermal and electrochemical stability made it the most sought-after, so most research focused on scientific research, and it was chosen as a metal layer in our current research.

Co3O4 belongs to the crystal structure of chiral cubic spinel of excess oxygen, which leads to p-type semiconductor behaviours with double direct band gaps (2,2ev -1,5ev) in the visible region of the spectrum. Co3O4 is defined as a mixed-valence antiferromagnetic material containing (Co+2, Co+3) Co+2 at tetrahedral sites and Co+3 at octahedral sites, The p-type semiconductor Co3O4 has been used as an excellent hole transport layer in solar cells.

Overall, the combination of p-type conductivity and direct optical energy gaps makes Co3O3 a promising material for application solar energy absorption, energy storage, catalysis , transition gas, and lithium-ion battery.

Several methods have been used to prepare Co3O4 films, including laser deposition , sol-gel method, chemical vapour deposition , and RF-sputtering .

2 Main results

Structural studies indicated that these films possess a spinel cubic structure preferentially orientated along the (111) direction.

The crystallite size diminishes with doping.

The optical transmittance of films improved to 63% for four wt% Bi-doped Co3O4

. The maximum conductivity value of 6.656(Ω cm)-1 was achieved for the eight wt. % Bi-doped Co3O4 films.

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Slepton production with a jet

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Abstract

A search for direct pair production of tau sleptons in final states with jets in MSSM of order LO. We will present an analysis based on proton-proton collision data at $\sqrt{s} = 7\,\text{Tev}$, $14\,\text{Tev}$ of interaction $pp \longrightarrow \tilde{\tau}\bar{\tilde{\tau}} + j$ at the Large Hadron Collider. The results obtained are interpreted by analyzing the variation of the hadronic cross section the hadronic cross-section as a function of $m_{\tilde{l}}$ and $\mu_F/m_{\tilde{l}}$.

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Impact of Co and Ni-doped zinc oxide nanoparticles on the optical characteristics of PS/ZnO nanocomposites thin films.
2024

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The study of the optical properties of polymer/ZnO nanocomposites has generated considerable interest due to their potential applications in optoelectronics [1]. These hybrid materials, composed of a polymer matrix and ZnO nanoparticles, offer a wide range of tunable properties, particularly in terms of light absorption, transmission, and emission [2].

In this paper, the optical properties of thin films of PS/ZnO were investigated as a function of the Co and Ni dopant elements of ZnO nanoparticles at a concentration of 10 wt%. The undoped and Co and Ni-doped ZnO nanoparticles were successfully synthesized using the co-precipitation method with dehydrated zinc acetate and sodium hydroxide as precursors. X-ray diffraction analysis confirmed the hexagonal structure of the obtained ZnO nanoparticles.

Thin polymer films were prepared using a simple spin-coating technique on glass slides by mixing ZnO nanoparticles with polystyrene (PS) polymer as the matrix. The pure ZnO and ZnO doped (Co and Ni) nanoparticles, at a concentration of 10 wt%, were used as fillers in the nanocomposites. Additionally, thin films of commercially available polystyrene were also prepared.

UV-Vis spectra characterization confirmed that the PS/ZnO nanocomposite thin films were highly transparent in the visible region and exhibited excellent UV-absorbing properties. The basic optical properties and optical constants of the PS/ZnO nanocomposites with thicknesses in the range of (526-710) nm were investigated. The transmittance and absorbance spectra were measured in the wavelength range of (300-900) nm.

The optical band gap Eg was determined; it was found that the Eg value of PS/ZnO10% Ni was the same as that of pure PS thin films, while it decreased for thin films of PS/ZnO and PS/ZnO 10% Co. The refractive index, which has a value of 1.017 for pure PS, was increased

in all the samples of PS/ZnO nanocomposites (pure and ZnO doped with Co and Ni), estimated to be between 1.87 and 1.96.

Keywords: nanoparticles, Co-precipitation, thin films, optical energy gap, refractive index.

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Structural and optical of CuO thin films deposited via spin coating: effect of cobalt doping

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Abstract

This study used the sol-gel spin-coating method to create Co-doped CuO thin films onto glass substrates. Copper (II) acetate monohydrate and cobalt (II) acetate tetrahydrate served as the initial salt ingredients, isopropanol functioned as the solvent, and monoethanolamine acted as a stabiliser. The as-coated films were dried at 250°C for 10 minutes, thereafter undergoing annealing at 500°C for one hour. X-ray diffraction (XRD) examination indicates that all films are polycrystalline and possess a monoclinic crystal structure. The average transmittance of the Co-doped CuO films exceeded 50%. The blue shift in the absorption edge of CuO with rising Co concentration in the film is significant, resulting in a reduction of the optical transmission breadth. In contrast, the two metrics, the band gap and refractive indices, showed an inverse trend, moving from 1.99 to 2.01 eV and from 2.13 to 2, respectively.

Keywords: Sol–Gel, Spin-Coating, Co-doped CuO films, XRD, Optical properties..

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Chalcocite (Cu_2S) semiconductor thin films for solar cells application: Influence of alkaline solution pH

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Copper sulphide (Cu_xS, x:1–2) semiconductor metal chalcogenides are actually investigated as prominent materials in the improvement of various applications in technology field. Chalcocite (Cu_2S) is amongst the most remarkable p-type copper sulphide used as chemical sensors, photocatalysis, cathode in secondary lithium batteries, energy storage devices, and principally as absorber thin films in solar cells.

In the present work, chalcocite (Cu_2S) thin films were prepared and characterized for their utilization as absorbers of light in solar cells. These thin films were elaborated on glass substrates at fixed temperature (40°C) and duration of deposition (6 hours) adopting the easiness and low-coast chemical bath deposition (CBD) technique. The bath contained aqueous solutions of copper sulfate ($CuSO_4.H_2O$) as copper source and thiourea ($CS(NH_2)_2$) as sulfur source. Aqueous ammonia (NH_3) and triethanolamine ($C_6H_{15}NO_3$) were added as complexant agents to the solution.

The influence of alkaline solution pH on the structural and optical properties of these films was investigated. Two principal characterization techniques were carried out to study the structural and optical properties of prepared films, X-ray diffraction technique (XRD) and UV-Vis-IR spectrophotometry. XRD analysis displayed the chalcocite phase, with polycrystalline monoclinic structure and five preferred orientations located at 9.55°, 18.97°, 24.82°, 28.71° and 29.60° corresponding to (110), (102), (212), (231) and (123) planes, respectively. The XRD peaks intensities were affected by the solution pH value; the lower and higher intensities were obtained at pH = 9 and 11, respectively. The crystallite size and crystal deformation values were estimated employing the Williamson-Hall (W-H) equation. The larger crystallite size (221 nm) and lower crystal deformation (24×10^{-4}) were found for chalcocite film deposited at pH = 11. Furthermore, optical band gap and Urbach energy have been investigated from optical transmittance spectra with wavelengths range (300–1800 nm). The transmittance of films was influenced by solution pH. All the prepared thin films showed a direct band gap which varied between 1.40–1.98 eV as a function of solution pH. The higher band gap and lower Urbach energy were obtained for pH = 11.

Our findings indicate that the chalcocite thin film deposited at pH = 11 is the most suitable as absorber light layer in solar cells compared to other prepared chalcocite thin films.

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Utilizing Invariant Theory for Exact Solutions of the Schrödinger Equation in Time-Dependent Hamiltonians: A Study of Quadratic and Linear Potentials

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The theory of invariants is an effective method to find the exact solution to the Schrödinger equation and study some time-dependent Hamiltonians associated with important physical systems like harmonic oscillators [1]. In this work, we addressed the study of special system physics with quadratic as well as linear time-dependent potential. This method is based on the relationship between the eigenstates of the invariant and the solution of the Schrödinger equation. These last two are linked by a time-dependent phase transformation for each eigenstates of an invariant such that the eigenfunctions becomes a solution of the Schrödinger equation while the phase is determined by a simple first-order differential equation [2-3].

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Synthesis and characterization of ternary mixed metal oxide based on Mg, Zn and Co for hydrogen storage using the sonochemical method

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The development of efficient hydrogen storage systems is crucial for the transition to clean energy technologies. Nanocomposites, comprising nanoparticles embedded in a matrix, offer a promising solution due to their enhanced physical and chemical properties [1]. Previous research has demonstrated that the grain size of nanocomposites significantly influences their hydrogen storage capacity, with smaller grains exhibiting improved absorption and desorption kinetics [2].

In this study, a simple method for synthesizing efficient ternary nanocomposite samples based on Mg, Zn and Co has been developed using the sonochimecal method. The nanoparticles obtained were characterized using structural methods. XRD diffraction confirmed the formation of different crystalline nanocomposite phases MgO, ZnO, and Co3O4, while Raman spectroscopy and FTIR identified the vibration modes and provided information on functional groups and chemical bands present in samples. Scanning electron microscopy (SEM) revealed an octahedral morphology of the nanoparticles.

The synthesized materials were evaluated for their hydrogen storage performance. The results indicated a promising hydrogen storage capacity of 0.55 Wt%, suggesting their potential as viable candidates for solid-state hydrogen storage applications. Further research is needed to optimize the composition and structure of these materials to achieve even higher storage capacities and improve their overall performance.

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Poster ☐

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First-principles study of the structural, electronic, optical, and photo-electrochemical properties of K2PtX6 (X = Cl, Br) compounds for green energy

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Solar energy harvesting is one of the most promising renewable energy resources, offering clean, non-toxic, and efficient energy from abundant and inexpensive materials. For a semiconductor to be used as a photocatalyst, its band structure must have suitably positioned conduction band minimum (CBM) and valence band maximum (VBM) to straddle the redox potential of water. Due to their remarkable optoelectronic and photovoltaic properties, halogenated perovskite-based compounds have attracted considerable attention for solar cell applications. In this work, we perform an in-depth analysis of the structural, electronic, optical, and photoelectrochemical properties of K_2PtX_6 (X = Cl, Br) compounds using first-principles calculations. Our results show that these materials exhibit favorable characteristics for light absorption and charge separation, making them promising candidates for green energy technologies. Using first-principles approaches, the calculated band gap energies are 3.39 eV and 2.66 eV for Rb_2PtBr_6 and Rb_2PtI_6, respectively. Employing the Tran-Blaha modified Becke-Johnson (mBJ) exchange potential, including spin-orbit coupling, yields more accurate results that are in good agreement with experimental measurements. The large difference in effective mass between electrons and holes enhances the separation of electron-hole pairs. Moreover, the optical analysis reveals that K_2PtX_6 (X = Cl, Br) perovskites possess a suitable band gap for absorbing visible light.
Keywords: Electronic Structure, Optical Properties, Photo-catalysis, Halogenated Perovskites, DFT Calculations.

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Indicate the topic of the presentation: First-principles study of the structural, electronic, optical, and photo-electrochemical properties of K2PtX6 (X = Cl, Br) compounds for green energy

- ✓ **Mathematics**

Numerical ODEs and Numerical PDEs (inc. BVPs)	Probability and Statistics

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Spectral analysis of Seyfert galaxies

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Active Galactic Nuclei (AGN) are highly energetic central regions of galaxies, powered by the accretion of material onto supermassive black holes. X-ray observations are a key tool for studying the complex processes occurring in AGN.

X-rays are produced in the accretion disk when ultraviolet (UV) and optical photons from the disk undergo inverse Compton scattering by thermal electrons in the hot corona. This primary X-ray emission forms a power-law spectrum. Additionally, a reflected X-ray component emerges when these primary X-rays irradiate the cooler accretion disk, resulting in further emission.

Several telescopes are dedicated to observing X-rays. In our research, we use data from both XMM-Newton and NuSTAR to study the spectral and timing properties of Seyfert galaxies. These joint observations offer broad energy coverage, enabling us to investigate features such as the soft X-ray excess below 3 keV, the iron Kα lines in the 6-7 keV range, and the Compton hump around 20-30 keV [1]. Moreover, studying X-ray variability in AGN provides a powerful diagnostic tool for probing their physical properties [2,3].

We analyze recent observations of several variable Seyfert galaxies. By performing spectral analysis using relativistic reflection models, we aim to constrain key astrophysical properties of the corona and the accretion disk surrounding the central supermassive black hole.

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Numerical study of two-dimensional natural convection in a hemispherical solar still

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Abstract

This paper deals with a numerical simulation of natural two-dimensional convection flows of an incompressible fluid with the Boussinesq approximation generated in a hemispherical solar still of radius R. The upper hemispherical transparent cover of the solar still is maintained at a constant temperature T_f and a concentration C_1, while the lower basin is at a temperature T_c and a concentration C_0, such that $T_c > T_f$ and $C_1 > C_0$.

We establish the heat and mass transfer equations and the boundary conditions associated with them, using the current-vorticity function formulation (ω–ψ)[1],[2],[3], the governing equations in dimensionless form are:

$$\frac{\partial^2\Psi^+}{\partial R^{+2}}+\frac{1}{R^{+2}}\frac{\partial^2\Psi^+}{\partial\theta^2}-\frac{cot\,\theta}{R^{+2}}\frac{\partial\Psi^+}{\partial\theta}=-R^+\Omega^+\sin\theta \quad (1)$$

$$\frac{\partial^2\Omega^+}{\partial R^{+2}}+\frac{2}{R^+}\frac{\partial\Omega^+}{\partial R^+}+\frac{1}{R^{+2}}\frac{\partial^2\Omega^+}{\partial\theta^2}+\frac{cot\,\theta}{R^{+2}}\frac{\partial\Omega^+}{\partial\theta}-\frac{\Omega^+}{R^{+2}sin^2\,\theta} \quad (2)$$

$$=\frac{1}{PrR^{+2}\sin\theta}\left(\frac{\partial\Psi^+}{\partial\theta}\frac{\partial\Omega^+}{\partial R^+}-\frac{\partial\Psi^+}{\partial R^+}\frac{\partial\Omega^+}{\partial\theta}-\frac{\Omega^+}{R^+}\frac{\partial\Psi^+}{\partial\theta}+\Omega^+cot\theta\frac{\partial\Psi^+}{\partial R^+}\right)$$

$$+Ra_t\left(\frac{sin\theta}{R^+}\left(\frac{\partial T^+}{\partial\theta}\right)-cos\theta\left(\frac{\partial T^+}{\partial R^+}\right)-\frac{cos\theta}{R^+}(T^+-1)\right)$$

$$+Ra_c\left(\frac{sin\theta}{R^+}\left(\frac{\partial C^+}{\partial\theta}\right)-cos\theta\left(\frac{\partial C^+}{\partial R^+}\right)-\frac{cos\theta}{R^+}(C^+-1)\right)$$

$$\frac{\partial^2T^+}{\partial R^{+2}}+\frac{1}{R^{+2}}\frac{\partial^2T^+}{\partial\theta^2}+\frac{2}{R^+}\frac{\partial T^+}{\partial R^+}+\frac{cot\,\theta}{R^{+2}}\frac{\partial T^+}{\partial\theta}=\frac{1}{R^{+2}\sin\theta}\left(\frac{\partial\Psi^+}{\partial\theta}\frac{\partial T^+}{\partial R^+}-\frac{\partial\Psi^+}{\partial R^+}\frac{\partial T^+}{\partial\theta}\right) \quad (3)$$

$$\frac{\partial^2C^+}{\partial R^{+2}}+\frac{1}{R^{+2}}\frac{\partial^2C^+}{\partial\theta^2}+\frac{2}{R^+}\frac{\partial C^+}{\partial R^+}+\frac{cot\,\theta}{R^{+2}}\frac{\partial C^+}{\partial\theta}=\frac{1}{LeR^{+2}\sin\theta}\left(\frac{\partial\Psi^+}{\partial\theta}\frac{\partial C^+}{\partial R^+}-\frac{\partial\Psi^+}{\partial R^+}\frac{\partial C^+}{\partial\theta}\right) \quad (4)$$

The numerical resolution of adimmensionalized differential equations is approached by the finite difference method. First of all, in order to validate our calculation code; our results were compared with those available in the literature. Good agreement is observed between our results and those of C. Chen et al [4] and N. Retiel et al [5].

All the results obtained relating to the effect of Lewis number (ratio between the thermal diffusivity and the solutal diffusivity), on heat and mass transfers. Lewis number varying between 0,2 and 5. A number of Pr =0,71 and a $Ra_t=10^4$. The thermal and solutal volume forces act in the same direction (N≥1)(figures 1, 2 and 3).

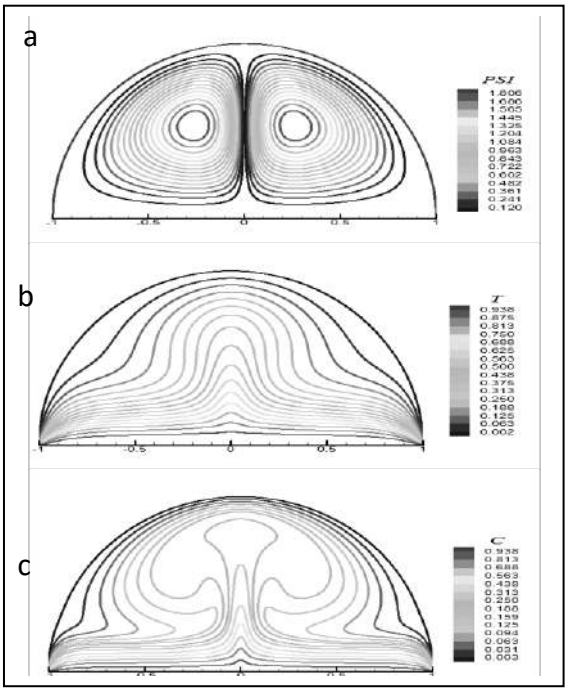


Fig-1: a)streamlines, b)isothermes et c)iso-concentrations for Le=0,2.

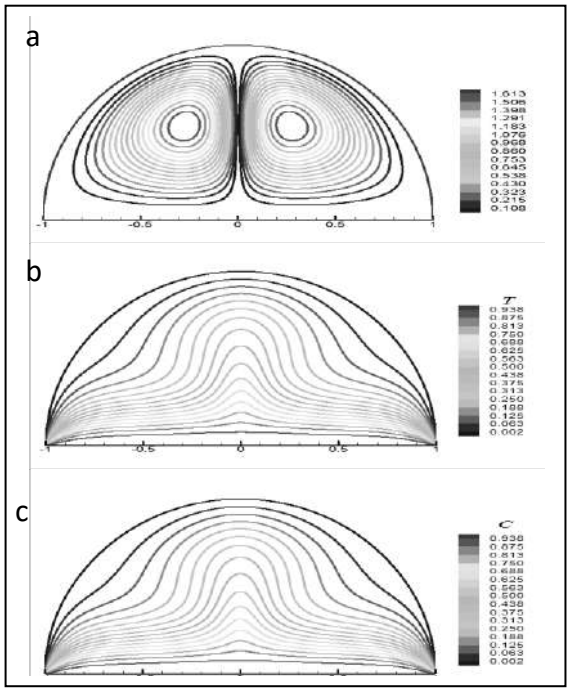


Fig-2 a) streamlines, b)isothermes and c)iso-concentrations for Le=1.

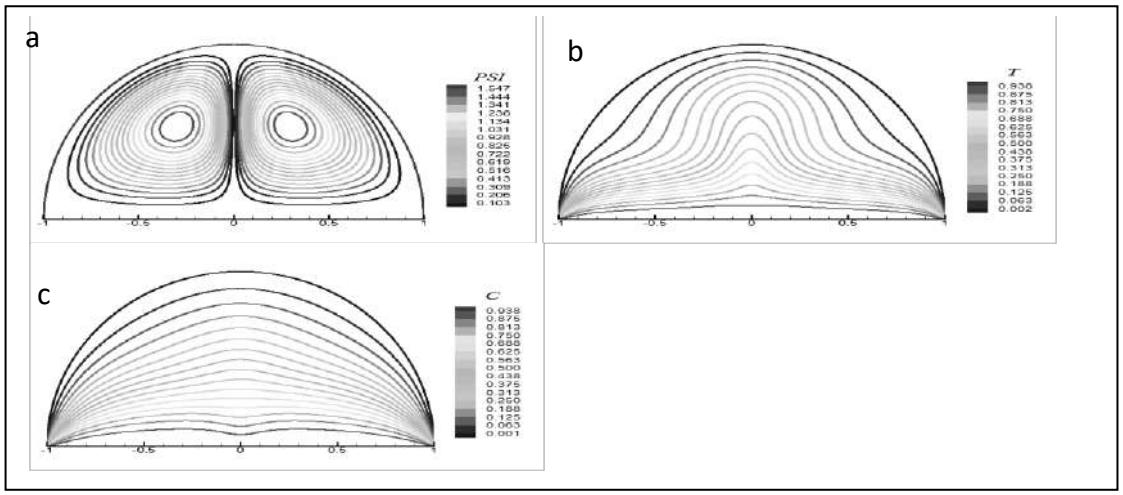


Fig.3 streamlines, b) isothermes and c) iso-concentrations, for Le=5.

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Influence of alumina on mechanical properties of triaxial ceramic

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Abstract

The aim of this work was to determine the effect of alumina on mechanical properties of triaxial ceramic. The basic composition was containing different contents of alumina (3, 5 and 8 wt%). It should be noticed here that all native raw materials are not against the environment. Samples were prepared by sintering the mixture at different temperatures (1140-1240 °C).

Subsequently, the obtained phases in the sintered samples were investigated by X-ray diffraction and Raman spectroscopy. The optimum sintering conditions gave a higher bulk density (2.50 $g.cm^{-3}$) and excellent mechanical properties.

The three point flexural strength of triaxial ceramic sintered at 1160 °C were 260 MPa.

The flexural strength value of this specimen is significantly higher than those reported for conventional ceramics.

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New Inner Product for Time-dependent non-Hermitian Systems

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Abstract

To solve the Schrödinger equation for a time-dependent non-Hermitian Hamiltonian, we use a time-dependent unitary transformation $F(t)$ to convert the time-dependent non-Hermitian Hamiltonian $H(t)$ into a time-independent pseudo-Hermitian Hamiltonian $\mathcal{H}^{PH}$, facilitating the solution of the initial system. We then define a new $\tilde{\eta}(t)$-inner product with $\tilde{\eta}(t) = F^{+}(t)\eta F(t)$ and show that the uncertainty relation remains real. A model of a particle with time-dependent mass subject to the action of a complex time-dependent linear potential is considered as an application.

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Neutron stars in scalar nonmetricity theories

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Abstract

Different formulations of General Relativity (GR) exist in flat spacetimes, attributing gravity either to torsion or non-metricity instead of curvature. This includes two additional geometrical representations of the same theory: teleparallel gravity and symmetric teleparallel gravity. Although, these formulations are dynamically equivalent, their modifications are not, leading to different phenomenological results. In this regard, our manuscript is dedicated to study the configuration of neutron stars in scalar tensor theories within the framework of symmetric teleparallelism, namely, scalar nonmetricity gravity. It consists of introducing non-minimal coupled scalar ϕ fields with nonmetricity scalar Q. We numerically solve the modified hydrostatic equations for both interior and exterior regions to extract the mass-radius relations. Our study has been carried out to investigate the compatibility of the obtained results with the observational constraints imposed by the gravitational waves (GWs) events and pulsar detections.

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Synthesis, crystal and molecular docking of methyl 2-(1,3-dithietan -2-ylidene)-3-oxobutanoate (MDYO)

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In this work, one of studied products by our group is the methyl 2-(1,3-dithietan -2- ylidene)-3-oxobutanoate.

This compound is one of the derivatives of ketene dithioacetal which evaluated as possible corrosion inhibitors of type 316L stainless steel in 1 M HCl solution, analysis of experimental results shows that MDYO inhibitor adsorb to the metal surface according to the Langmuir model and the mechanism of adsorption of this inhibitor involve physisorption [1]. MDYO has also a high capacity to inhibit copper corrosion in nitric acid solutions [2].

The methyl 2-(1,3-dithietan-2-ylidene)-3-oxobutanoate (MDYO) was synthesized as follows: K2CO3 (42 g, 0.3 mol) and methyl acetoacetate (0.1 mol) in 50 mL of DMF were agitated magnetically. Carbon disulfide (9 mL, 0.15 mol) was added, and the agitation was maintained for 10 min before adding Diiodomethane (0.12 mol), drop by drop for 20 min. After 7 hours of agitation at room temperature, ice water (500 mL) was added to the reaction mixture. The precipitate formed was filtered, dried, and recrystallized in ethanol. White crystals were obtained for the product prepared.

The title compound, C7H8O3S2, crystallizes in the P21 space group of the monoclinic system with two molecules per unit cell.The C2S2 ring is close to planar and the dihedral angle between the mean planes of 1,3-dithietane rings and the mean planes of the methyl oxobutanoate group is 3.87º which means the flatness of the molecule. Short intramolecular S…O contacts occur 2.622Å stabilizes the molecular structure. In the crystal molecules stack head-to-tail in columns along the a-axis direction. The columns are linked via C—H…O and C—H…S hydrogen bonds s, forming layers parallel to the bc plane. The layers are linked via weak interactions C—H…π and π-π, forming a three-dimensional network.

Molecular docking calculations were performed with Autodock Vina [3]. The Chimera program was used for the preparation of the target protein and ligand molecules [4], and the interactions between receptor and ligand molecules were visualized using BIOVIA Discovery Studio Visualizer v21 (Biovia DSV 2021) [5]. The human enzyme was obtained from RCSB Protein Data Bank (PDB: 4EY6). Chimera software defined the active sites as a box, was centered on (-10.49, -44.02, 30.13) coordinates and sized to (12.63× 9.03 × 12.70) $Å^3$. As a ligand, the PDB file repre-senting MDYO was generated from its optimized structure, which was calculated using the B3LYP/6-311G (d, p).

Molecular docking technology in predicting the main active target of treatment in Nonalcoholic Fatty Liver Disease (NAFLD) [6].

Keyword : *Ketene Dithioacetal Derivatives, DRX, Molecular docking***.**

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Pulsed Laser Deposited of ZnO thin films Study of the substrates nature

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ABSTRACT: Pulsed laser deposition technique (PLD) is used to synthesis a polycrystalline zinc oxide (ZnO) thin films onto glass and silicon substrates at 450°C. The used source is a KrF excimer laser (248 nm, 25 ns, 5 Hz, 2 J/cm2).

The effects of glass and silicon substrates on structural and optical properties of ZnO films have been investigated. X-ray diffraction patterns show that ZnO films are polycrystalline with a hexagonal wurtzite type structure with a strong (103) orientation, with a good crystallinity on monocrystalline Si (100) substrate.

The grain sizes calculated from XRD patterns varie from 26 to 15 nm. All the films have a good surface morphology. In order to study the optical properties of ZnO films, the M-lines technique is employed. The distinct M-lines of the guided transverse magnetic (TM) and transverse electric (TE) modes of the ZnO films waveguide are observed; and based on them, refractive index and film thickness are measured.

Optical transmission spectra show a good transparency in the visible range and the calculated optical band gap is equal to 3.22 eV.

KEYWORDS: Pulsed laser deposition, Thin films, ZnO, Waveguiding properties.

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Gamma-ray emission cross sections measurement using AFRODITE detector system

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This study focuses on the use of the AFRODITE (AFrican Omnipurpose Detector for Innovative Techniques and Experiments) spectrometer to measure nuclear gamma-rays emission cross sections from iron (Fe) targets bombarded with protons. AFRODITE, housed at iThemba LABS (Cape Town, South Africa), features a rhombicuboctahedral structure with 16 detector slots. For this experiment, eight Clover-type high-purity germanium (HPGe) detectors were employed, ensuring high-efficiency detection of both high- and low-energy gamma photons. The clovers were placed in a fixed geometry with four detectors at 90° and four at 135° relative to the incident beam direction. The system provides optimal coverage and resolution for capturing gamma rays emitted during nuclear reactions.

The iron targets were bombarded with 125 MeV proton beam delivered by the separate-sector cyclotron of iThemba LABS. This energy is significant in studying prominent nuclear deexcitation gamma-lines produced during solar flares. The proton beam induced gamma emissions that were recorded and analyzed using the AFRODITE detector array.

In this work, we report our new cross sections data measured for the production of the gamma-lines of energies between 126 and 1480 keV. Our data consistently extend to higher proton
energies and then enriches the database. The results constitute valuable data for refining theoretical models and improving our knowledge of proton-induced nuclear reactions on iron.

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Effect of drying temperature on the structural, morphological and optical properties of sol-gel synthetized ZnO thin films

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Abstract

In the field of optoelectronics, most applications require high-quality thin films with good properties to achieve higher productivity. Therefore, this study is based on improving the quality of thin films prepared by sol-gel method. Zinc oxide (ZnO) thin films were successfully synthetized by sol-gel dip-coating method. The effect of drying temperature (150, 200, 300 and 400 ° C) on the structural, morphological and optical properties of deposited thin films of ZnO was studied by using X-ray diffractometer, atomic force microscopy and UV-Visible spectrophotometer, respectively. XRD patterns reveal that all samples possess the hexagonal wurtzite structure with two predominant growth orientations (002) and (103). The crystallite size was decreased from 21.63 to 15.50 nm. AFM images show that the increase in the drying temperature leads to an increase in the grain size from 92 to 122 nm and a decrease in the RMS roughness from 33 to 12 nm, indicating the improvement in the surface quality of films. UV-Vis transmittance spectra showed that all the films are highly transparent in the visible region (~ 80 %). Moreover, the optical band gap energy was found to decrease from 3.27 to 3.23 eV with increasing drying temperature, and this decrease can be attributed to the increase in free carriers concentration due to the increase in disturbed oxygen vacancies at high drying temperature. Finally, the results of this study show that a high drying temperature led to obtaining thin films with high quality.

Key words: Zinc oxide, Sol-gel, Thin films, optoelectronics, XRD.

1. Introduction

Among the metal oxides, sol-gel synthetized ZnO thin films is a promising semiconductor material, characterized by high piezoelectricity, high exciton binding energy (60 meV) and wide-bandgap (3.37 eV), as well as ZnO is biologically safe and biocompatible **[1]**. Therefore, these features are the main reasons that ZnO has become widely available in many applications. To prepare high quality thin films, we will try to find the appropriate drying temperature. The drying temperature is used in the sol-gel curing between subsequent layers. This is done to evaporate the solvent and remove most of the organic compounds. Most publications used only one or two drying temperatures **[2]**. In this study, the effect of drying temperature on the physical properties of ZnO thin films was investigated.

2. Materials and method

ZnO thin films were synthetized on glass substrate by sol-gel dip-coating method, using zinc acetate dehydrate, ethanol, and MEA. The mixture was stirred at 60 ° C for 2 h. The films were deposited by using a computer-controlled dip-coater. Then, the films were dried at different

temperatures (150, 200, 250 and 300 °C) after each dipping operation. Finally, the films were annealed at 500 °C for 2 h.

3. Results and discussion

Fig.1(a) shows that all the samples have hexagonal wurtzite structure of ZnO with two predominant peaks (002) and (103). As the drying temperature increases, the intensity of the peaks increases, indicating an improvement in the crystalline quality of the films. Fig.1(b) shows that the grain size increased from 92 to 122 nm and the RMS roughness decreased from 33 to 12 nm with the increase in drying temperature, indicating the improvement in the surface quality of the thin films. Fig.2(a) shows the transmittance spectra of ZnO, the films are highly transparent in the visible region (80-90%). The Tauc plot of transmittance was used to obtain the optical bandgap energy of ZnO. From Fig.2(b), it was found that the gap decreased from 3.27 to 3.23 eV with increasing drying temperature.

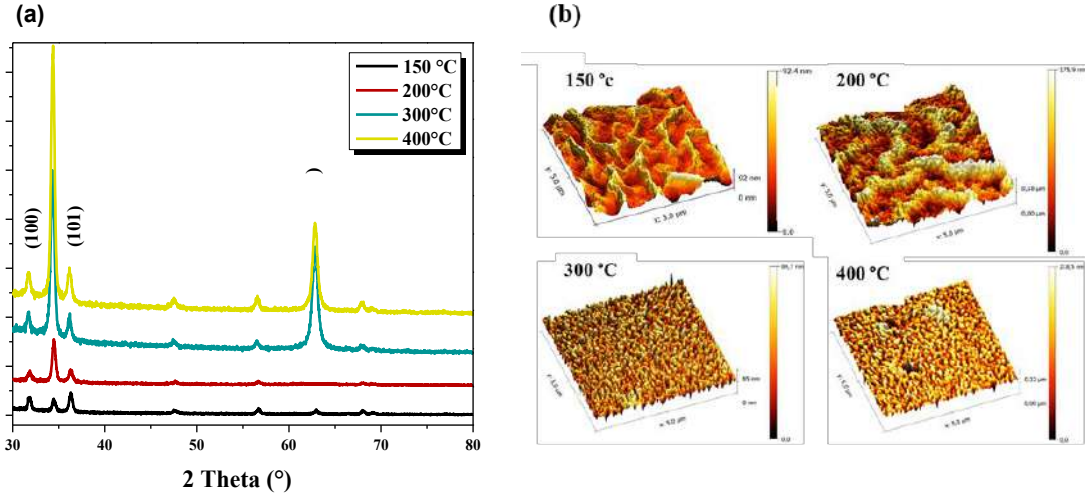


Fig.1. (a): X-ray diffraction patterns of ZnO thin films dried at different temperatures: 150 °C, 200 °C, 300 °C and 400 °C. **(b):** 3D AFM images of ZnO thin films dried at different temperatures.

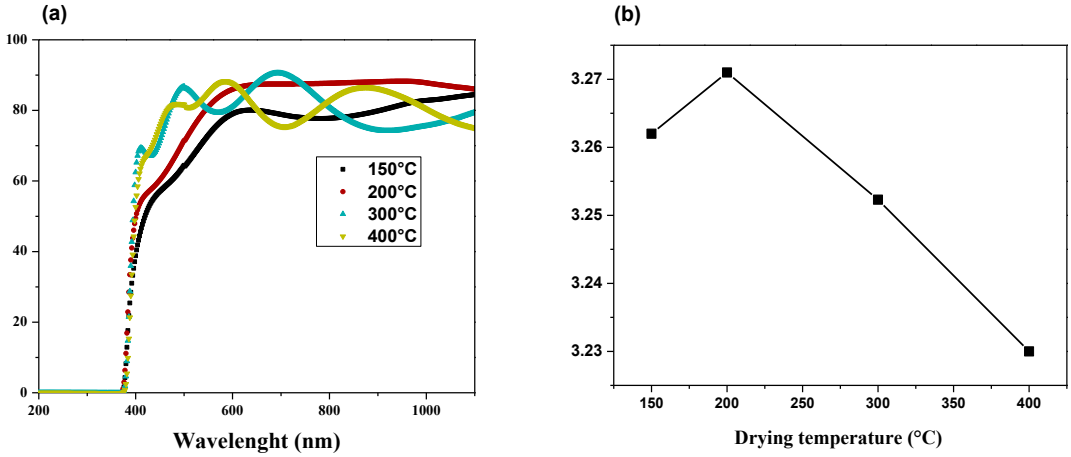


Fig.2. (a): Optical transmission spectra of ZnO thin films dried at different temperatures: 150 °C, 200 °C, 300 °C and 400 °C. **(b):** Effect of drying temperature on the bandgap energy of ZnO.

4. Conclusion

The results of this study show that a high drying temperature (300 °C and 400 °C) led to obtaining a ZnO thin films with high quality.

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Triple differential cross sections for electron impact ionization of Ar (3p) in the coplanar symmetric geometry

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The investigation into single ionization induced by electron impact on molecules and atoms stands as a cornerstone in the realm of fundamental collision studies, offering indispen-sable insights. Its pertinence extends across diverse fields of physics.

Here we calculate triple differential cross sections(TDCS) for the electron impact ionization of argon(3p) in coplanar symmetric geometry at various incident electron energies (Fig.1 presents a representative case where the incident electron energies is 85.8 eV), using two models: 2CWZ model and 3CWZ model . Within this 2 models, the ejected electrons are represented by Coulomb waves with variable charges Z(r) instead of an effective charge while the incident electron is described by a plane wave in 2CWZ model and a coulomb wave with variable charge in 3CWZ model; taking into account the post collision interaction (PCI). The results are compared to the experimental data of Nixon and Murray [4].

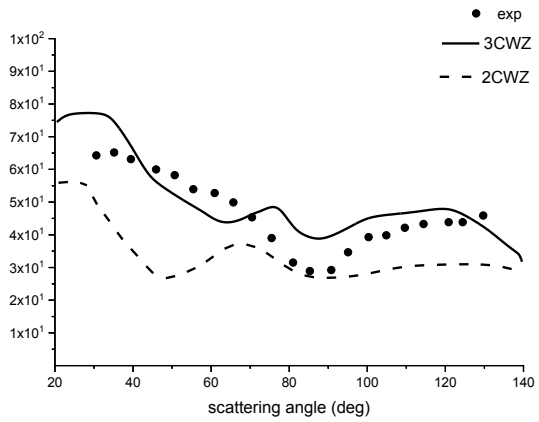


Fig.1.TDCS of Argon atom as a function of scattering angle θ in the coplanar symmetric geometry at the incident electron energie of 85.8 eV and the two ejected electrons $E_1 = E_2 = 35\ eV$. Solid circles are the experimental data of Nixon and Murray [4].

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Numerical study of natural convection in a porous medium saturated with a non-Newtonian nanofluid under the influence of a magnetic field

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This research delves into the intricate interplay between magnetic fields, nanotechnology, and porous media by numerically investigating the impact of a magnetic field on natural convection within an inclined square porous cavity filled with a non-Newtonian nanofluid. The nanofluid, composed of water and single-wall carbon nanotubes (SWCNTs), exhibits non-Newtonian behavior, which is modelled using the power-law model. The cavity's side walls are thermally insulated maintained, while the top and bottom walls are at different temperatures.

A finite difference method is employed to solve the governing equations, which account for the effects of the Rayleigh number, Hartmann number, SWCNT volume fraction, and inclination angle on the fluid flow and heat transfer characteristics within the porous medium.

Our findings reveal that increasing the concentration of SWCNTs significantly enhances heat transfer, despite the increase in fluid viscosity. Furthermore, the power-law index and the Hartmann number play pivotal roles in determining the strength of fluid flow and the rate of heat convection. An inclination angle of 60 degrees emerges as the optimal configuration for maximizing heat transfer.

This study provides valuable insights into the complex interactions between magnetic fields, nanofluids, and porous media, offering potential applications in various fields, including thermal management systems, energy storage, and biomedical engineering.

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Optical Properties of Chalcogenide CFTS Thin Films Grown by Thermal Evaporation

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Abstract

Photovoltaic cells play a crucial role in the global transition towards a renewable energy-based economy, providing a clean and competitive energy source. Copper, iron, and tin chalcogenides (CFTS) are emerging as promising materials for solar cells, offering energy efficiency comparable to established technologies. Despite persistent challenges, ongoing research on CFTS paves the way for more efficient and environmentally friendly solar energy. Our study focuses on the development and understanding of the properties of chalcogenide materials, particularly CFTS, in thin-film form. We fabricate these thin films through vacuum thermal evaporation and investigate their optical properties, especially refractive index, n_c, and thickness, d, based on spectrophotometry. Additionally, we analyze the effect of thickness on the transmittance of CFTS thin films.

Keywords: Chalcogenides Thin Films CFTS, Optical Characterization, Optical Properties.

1 Introduction

The chalcogenide material Cu_2FeSnS_4 in thin films, CFTS, presents considerable interest due to its semiconductor properties and its potential applications in various technological fields, particularly in photovoltaics, catalysis, and optoelectronics [1, 2]. The objective of this work is to deepen our understanding of the optical characteristics of this compound Cu_2FeSnS_4. To achieve this goal, we rely on a series of optical characterization techniques to thoroughly explore the interactions of light with Cu_2FeSnS_4.

2 Mainresults

Optical characterization is a method used to study the interactions between light and matter. It offers a detailed overview of the optical properties of materials, such as absorption, reflection, and transmission. UV/Visible spectrophotometry is based on the interaction of electromagnetic radiation and material in the range extending from near UV to very near IR, either between 300 and 1800 nm. This part of the spectrum is relatively poor in information on the structure of molecular compounds. On the other hand, the absorbance of near-UV and visible compounds is used in quantitative analysis by application of the theoretical law of Beer-Lambert. This device allowed us to plot curves representing the variation of transmittance, T, and reflectance, R, of CFTS thin films prepared by thermal evaporation, as a function of wavelength, λ, in the infrared spectral range, covering a range from 300 to 1800 nm (Figures 1 & 2). By exploiting these curves, we can calculate the refractive index, n_c, (equation 1) and estimate the thickness, d, (equation 2) of the CFTS thin films [3, 4]. Moreover, the possibility to determine different optical properties, such as the optical absorption threshold, the absorption coefficient, α, the band gap width, Eg, the Urbach energy, Er, …etc.

$$n_c = \left(n_s \cdot \frac{1+\sqrt{R_{max}}}{1-\sqrt{R_{max}}}\right)^{1/2} \quad \text{(Equation 1)}$$

With :

n_c: refractive index of a thin layer.

n_s: refractive index of the substrate (glass: equal to 1.5).

R_{max}: maximum reflectance of the chosen fringe.

$$d = \frac{(p+1).\lambda_2}{2.n_c} \quad \text{(Equation 2)}$$

With : $p = \frac{\lambda_2}{\lambda_2 - \lambda_1}$

Where :

d : thickness of the thin layer.

λ_1 and λ_2 : wavelengths of two successive fringes.

n_c : refractive index of the thin layer

P : fixed integer number, even or odd.

Therefore, the values of the refractive index, n_c, of the CFTS thin films are approximated to n_{cmoy}=1,82 (figure 3) which are almost identical for the elaborate CFTS thin films and they are in good agreement with the values found in the literature. Furthermore, the determination of the thicknesses, d, of the CFTS layers shows that the values found are in good agreement with the theoretical method applied, where the thicknesses vary from 824.73nm to 1463.13nm (figure 4). Finally, the study of the effect of thickness on the transmittance, d (T), of CFTS thin films, presents a weak linear decrease of T with the increase of d. In addition, the thicknesses of our layers do not influence the transmission of the prepared CFTS films shown by the low slope presented by the linear fitting (figure 5).

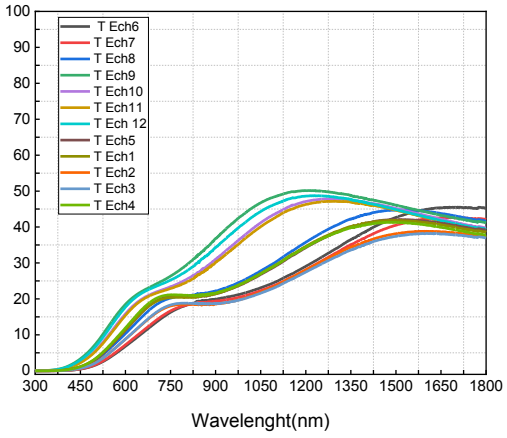


Figure 1: Grouping of the Transmittance spectra of the 12 CFTS thin films as a function of the UV-Visible wavelength.

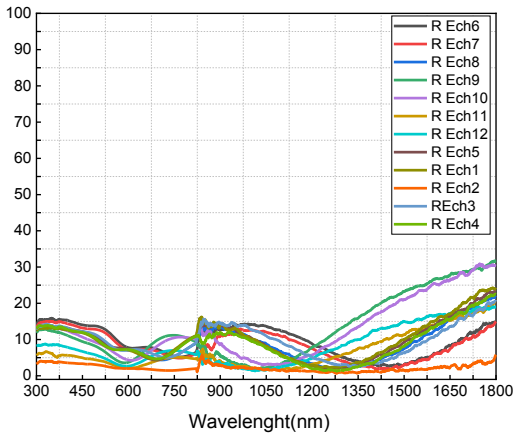


Figure 2: Grouping of the Reflectance spectra of the 12 CFTS thin films as a function of the UV-Visible wavelength.

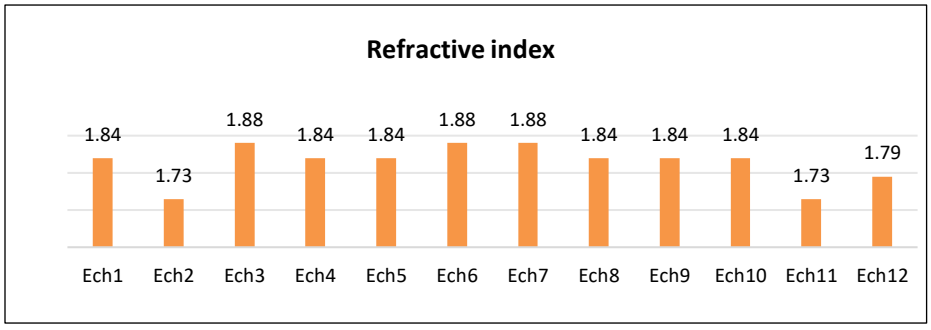


Figure 3: Histograms of the refractive index values of Cu_2FeSnS_4 thin films prepared by vacuum thermal evaporation.

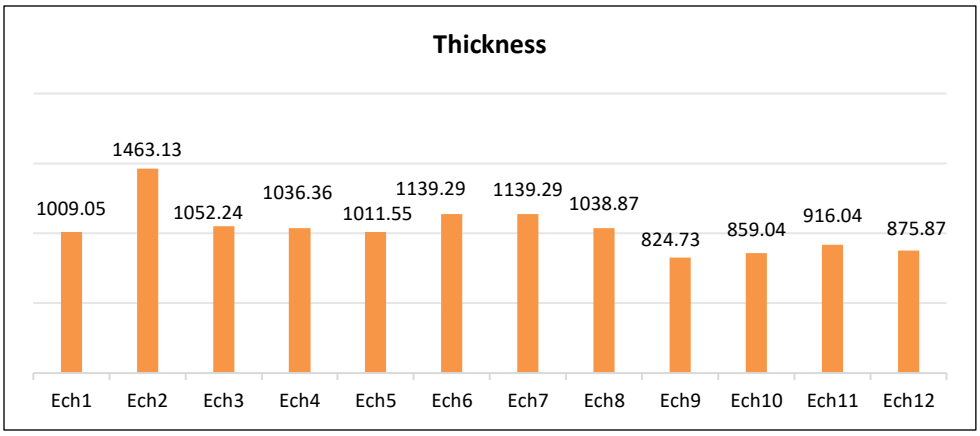


Figure 4: Histograms of the thickness values of Cu_2FeSnS_4 thin films prepared by vacuum thermal evaporation.

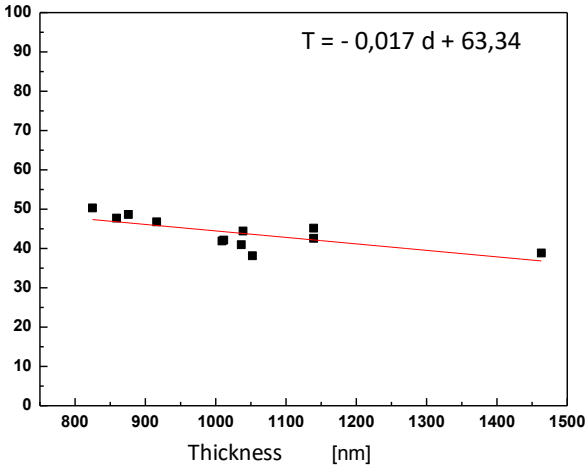


Figure 5: Effect of the thickness of Cu_2FeSnS_4 thin films prepared by thermal evaporation under vacuum on transmittance.

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Influence of magnetic field on nonlocal resonance behavior in perforated Levinson nanobeams with periodic square holes

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In this paper, we explore the effects of magnetic field and small-scale influences on the dynamic vibrations of a simply supported nanobeam structure. The structure under study is composed of a rectangular configuration longitudinally perforated with a periodic network of square holes, and it is exposed to an axial magnetic field [1]. The investigation employs both the Euler–Bernoulli beam model (EBM) and the Levinson beam model (LBM), two commonly recognized theories in beam mechanics.

We derive the resonance frequency expressions by modifying standard equations for dynamic nanobeam vibration. Maxwell's equations are used to express how the applied magnetic field was influenced [2]. The small-scale impacts, which become critical at the nanoscale, are incorporated by employing Eringen's nonlocal theory. This theory accounts for the impact of small material length scales, which are frequently overlooked in traditional elasticity theories. By taking into account these nonlocal effects, the accuracy of vibration analysis improves dramatically, particularly when predicting the behavior of nanostructures [3].

The Navier-type solution method, an analytical approach, is employed to solve the coupled governing equations, enabling us to yield the perforated nanobeam's resonance frequency. Numerical results show that numerous factors, including the intensity of the magnetic field and the small-scale impact, influence the resonance frequency. In addition, we found that the geometric parameters of the nanostructure, such as the size and number of holes, play an important role in affecting the resonance frequency. Changes in the size and number of holes in the nanobeam cause a noticeable shift to occur in resonance frequencies, which are impacted by the magnetic fields. The small-scale effect, modeled via Eringen's nonlocal theory, further impacts this variation, in particular at nanometric dimensions.

The numerical results obtained are thoroughly discussed. New insights are given that can provide the appropriate design and improve micro- and nano-electromechanical systems (M/NEMS). The research presented a thorough understanding of how longitudinally perforated nanobeams respond to different external stimuli, which is critical for the development of more effective and reliable nanoscale devices.

Keywords: Longitudinally perforated, Small-scale effect, Magnetic field, Resonance frequency

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Spin-1/2 particle confined to a surface in presence static magnetic field.

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Abstract :

In this work, we will discuss the fundamental framework of the thin-layer method for a non-relativistic particle of spin-1/2 on a curved surface. After a short review of the Schrödinger-Dirac equation in a curved space-time, we have applied the thin-layer quantization scheme on the confined particle using the non-relativistic limit of the letter equation. This procedure defines dynamics in the space-time very close to the surface, where we have introduced the squeezing potential as minimal coupling. To split the wave function into a normal and a tangential part, we have supposed that the Fock-Ivanenko coefficient $\Gamma_3=0$. As a result, we have obtained a new scalar geometric potential and composed of three terms come from the confining process. We have also shown the important role of the coupling between the geometry of the curved surface and the spin of the particle in creating bound states

It would be important to consider a constant magnetic field applied to confined two-dimensional electron gas, and to look at the impact of the above geometric potential on Landau levels and on Hall conductivity. This task is under consideration.

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Dynamic Response Assessment of a Double Nanobeams System under Nanoparticle Adsorption Influence

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Abstract

This paper investigated the impact of nanoparticle loads on the dynamics response of a double FGM porous nanobeams (DFGPNB) connected by an elastic medium based on the Euler–Bernoulli beam model (EBM). Lennard-Jones (6-12) potential determined the adsorption-induced energy owing to van der Waals (vdW) interaction mechanism between adatom-adatom/substrate. Nonlocal frequency shift expressions were derived by modifying the standard equations of dynamics beam vibration. The small-scale effect was adopted via nonlocal strain gradient elasticity theory (NSGT). Also, the motion equation of the entire system was obtained and solved with a numerical approach DQM to determine a frequency shift of DFGPNB. Therefore, numerical results showed that the nonlocal frequency shift depends on the nonlocal parameters, spring parameter, adsorption density, porosity volume fraction, and power-low index. Thus, numerical results are discussed in detail for a proper analysis of the dynamic behavior of adatoms-nanobeam systems, which are of interest in developing mass-sensing integrated devices.

Keywords: nonlocal frequency shift, double FGP nanobeams, adsorption-induced energy, van der Waals (vdW) interaction, DQM

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Characterization and studying of ZnO thin films deposited by spray pyrolysis: Effect of Deposition Time

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Zinc oxide thin films have gained significant attention over the past three decades due to their electro-optical properties, making them suitable for various optoelectronic applications [1]. These films can serve as transparent and conductive window layers in thin film solar cells, and ZnO is often utilized as a transparent conductive oxide (TCO) layer in different types of thin film silicon solar cells, functioning as either a front or back contact [2]. Numerous studies have examined the structural, optical, morphological, electrical, and physical properties of ZnO thin films produced through various deposition methods [3,4]. In this study, we employed the spray pyrolysis technique to deposit ZnO thin films. Despite the deposition method used, the effects of deposition time an area of active research. Given the diverse applications of ZnO-based devices, investigating how their properties change with this parameter is crucial.

In this study, zinc oxide thin films were prepared using the spray pyrolysis technique. A series of ZnO films were deposited on glass substrates at 400 °C, with deposition times varying from 2 to 10 minutes. The precursor solution consisted of zinc acetate dissolved in distilled water at a concentration of 0.1 molarity. The structural, optical and electrical properties of the films were analyzed using X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy and electrical DC transport characterization. The XRD patterns indicated a polycrystalline hexagonal wurtzite structure, with a preferred orientation along the (002) plane. The ZnO thin films exhibited high transparency in the visible spectrum, achieving a maximum transmittance of 90%, while the optical band gap was determined to be between 3.32 and 3.56 eV. ZnO thin films deposited at 10 min exhibit all the necessary properties for solar cell production. These films demonstrate reduced thickness, improved crystallinity, enhanced transmittance, and a wide band gap, indicating that these conditions are optimal for creating ZnO thin films intended for use as transparent conductive oxide (TCO) layers in solar cells.

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Nuclear structure properties of odd-even Proton rich In isotopes

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Instable systems nearby proton drip-line have important contributions and a significant influence on the theoretical and experimental knowledge progress [1]. In order to understand the nuclear properties, shell model theory have been considered to interpret and develop the two body matrix elements of N-N interaction. Moreover, the interactions between nucleons in different orbits lead to modifications on shell structure, therefore to the appearance of possible new magic numbers. The consideration of this effect may offer the opportunity to predict some missed nuclear structure properties, in non-investigated systems.

With the aim of reproducing the nuclear structure properties of odd-even Z=49 isobars; we have performed calculations, by means of NuShellX@MSU [2] nuclear structure code, using recent experimental single particle energies [3]. The two-body matrix elements (TBMEs) of the used effective interaction in Ni core were deduced from those of *sn100pn* realistic one in ^{100}Sn mass region [4]. Basing on the original interaction, the TBMEs are then modified taking into account the similarity effect and the monopole interaction [5] in ^{56}Ni to introduce ni56pn new interaction. The obtained results are then compared to the available experimental data.

Keywords: Z=49 isobars, Proton drip line, Nuclear Structure Spectroscopy, NuShellX@MSU nuclear structure code, Gamma Decay.

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Hawking temperature of the non-commutative Anti-de Sitter Schwarzschild black hole

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Abstract

In this study, we investigate the impact of non-commutative (NC) geometry [1] on the Hawking temperature [2] of the Anti-de Sitter Schwarzschild black hole [3]. First, we derive the NC correction to the metric $\hat{g}_{\mu\nu}(r,\Theta)$ to leading order in NC parameter Θ. The resulting deformed metric allows us to compute the modified event horizon within this geometry. Using these results, we obtain the NC correction to the Hawking temperature up to second order in Θ. Our findings show that NC geometry removes the divergence of the Hawking temperature at the final stage of black hole evaporation. Moreover, the combined effect of non-commutativity and the cosmological constant introduces a new temperature profile characterized by both minimum and maximum temperatures, indicating the presence of two distinct phase transitions. By interpreting the cosmological constant as an effective pressure acting on this black hole [4], we estimate the NC parameter for a given pressure, finding it to be of the order of 10^{-35} m. This result suggests that the quantum properties of spacetime become significant at the Planck scale.

Keywords: Non-commutative geometry; Anti-de Sitter Schwarzschild black hole, Hawking temperature

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Plastic instabilities and associated parameters in the presence of dynamic strain aging in an Al-Mg alloy

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Jerky flow or the Portevin-Le Chatelier (PLC) effect is one of the most striking manifestations of plastic instability. This unstable plastic flow is due to the dynamic strain aging (DSA) mechanism, which results from the interaction between solute atoms and mobile dislocations. Solute atoms diffuse to and age mobiles dislocations during their temporary arrests at local obstacles (forest dislocations, precipitates, etc). Hence, DSA reduces the strain rate sensitivity of the flow stress, which may become negative in some range of temperature, strain and strain rate.

This work is devoted to the uniaxial tensile characterization of the PLC effect in an Al-2.5%Mg alloy in a wide range of applied strain rates at room temperature. We analyze effects of strain and strain rate on the characteristic parameters of the unstable plastic flow. It is shown that the appearance and the amplitude of the resulted instabilities depend on the imposed strain rate and on the strain level. The critical plastic strain, beyond which the PLC phenomenon appears, increases with the strain rate at high strain rates (behavior known as normal). An opposite behavior is observed at low strain rates (behavior known as inverse). These results are interpreted in accordance with the DSA mechanism which plays a crucial role in the plastic deformation of Al-Mg alloys.

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Free Vibration Analysis of Hybrid Composite Plates reinforced with Carbon Nanotubes and Graphene Nanoplatelets.

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Abstract

This paper presents the Free Vibration Analysis of Hybrid Composite Plates reinforced with Carbon Nanotubes "CNTs" and Graphene Nano platelets "GPLs". The material properties of CNTs are determined using the mixing rule, while the GPLs is using the Halpin-Tsai and voigt-Ress micromechanical model. In addition, the finite element method is employed to discretize the plate into sixty-four elements. This work starts by mentioning a validation of the non-dimensional natural frequencies of a composite plate reinforced by four types of functionally graded carbon Nano-tube configurations: i) uniform distribution, ii) X distribution shape, iii) O and A distribution. Next, a proposed hybrid composite plate reinforced by CNTs and GPLs is considered to study the free vibration analysis, taking into account the effect of oriented nanotubes.

Keyword

Free Vibration Analysis; Carbon Nano-tubes; Graphene Platelets; Hybrid Composite Plates; Functionally Graded Distribution.

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Modeling Vibrations of Gold Nanobeams: Impact of Hydrogen Adatoms and Structural Design

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Abstract

To contribute to the field of nanomaterials, frequency shift calculations were employed to study and model the vibrations of a gold nanobeam system. This system is characterized by periodic square holes along the nanobeam, as well as the adsorption of hydrogen adatoms on its surface. The Euler Beam Model (EBM), developed by modifying the coupled system equations and incorporating small-scale behavior via Eringen's elasticity theory, was utilized alongside the Shear Beam Model (SBM). To account for the total energy shift, van der Waals (vdW) interactions were considered, introducing both adatom-substrate and adatom-adatom energies based on the Lennard-Jones potential (6–12). The frequency shift for the H/Au(100) system was calculated and found to be influenced by factors such as the size, number, and dimensions of the nanobeams, as well as the adsorption density and mode number. A comprehensive analysis of these results has provided valuable insights for the optimal design of mass detection and biosensor devices, with potential applications in nanotechnology.

Keywords: Nanomaterials, Frequency shift, Gold nanobeam, Hydrogen adsorption, Van der Waals interactions

1 Introduction

Nanotechnology has emerged as a crucial field of study with numerous applications in modern technology. Among these applications is the study of vibrations in adatom-nanobeam systems, which are widely employed in small-scale, cost-effective mechanical devices designed for mass-sensing. These systems have attracted considerable attention due to their notable advantages, such as enhanced reliability, rapid response times, and high sensitivity, making them central to advancements in nanotechnology research [1].

In this study, we integrate interaction potential with traditional beam vibration theories and Eringen's elasticity theory to investigate the dynamic behavior of nanobeams with dispersed adatoms. By incorporating both bending and shear stiffness, we develop shear and Euler beam models, considering the Lennard-Jones (6–12) potential and the impact of van der Waals (vdW) interaction energy. The objective is to provide a deeper understanding of the vibration characteristics of these nanoscale systems [1].

2 Problem formulation

As shown in Fig. 1a, we assume a nanostructure with dimensions of length L, width b, and thickness $2h$ that is perforated with a network of periodic square holes with spatial period (s_p) and size (d_h). In Fig. 1b, we define $\alpha = 1-(dh/sP)$ as the hole size ratio spanning from 0 to 1 (complete structure) and N as the number of holes along the section.

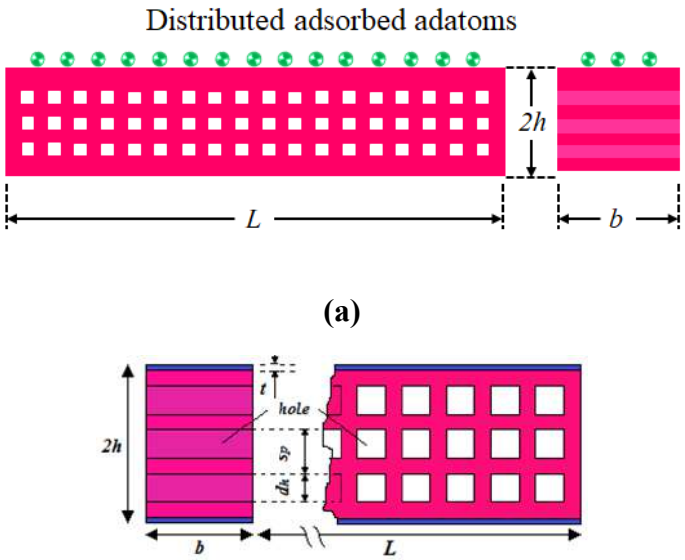


Fig 1. Models of the adatom-nanobeam system include: (a) a perforated nanobeam in which the adatoms are dispersed; and (b) a nanobeam geometry including a periodic network of square holes.

3 Results and discussion

For a nanostructure made of Au (100) with the geometry (L,b,h)=(100nm,20nm,10nm), we calculated the non-local vibration frequency shift by varying the filling ratio, the number of square holes, the density of dispersed adatoms, and the nanobeam thickness. The characteristics of the material were (e_0a)=0.2L, K=5/6, ρ=19300$kg/m3$, and E=78600MPa.

As we can see in Fig. 2, the impact of the shear modulus (AG_{eq}) causes EBM to move away from SBM when the filling ratio drops and towards SBM when the filling ratio increases. Regarding Fig. 3, the presence of holes causes the difference between the two approaches to rise because of the increased shear effect. In this case, EBM and SBM are near to each other when holes are missing [1-2].

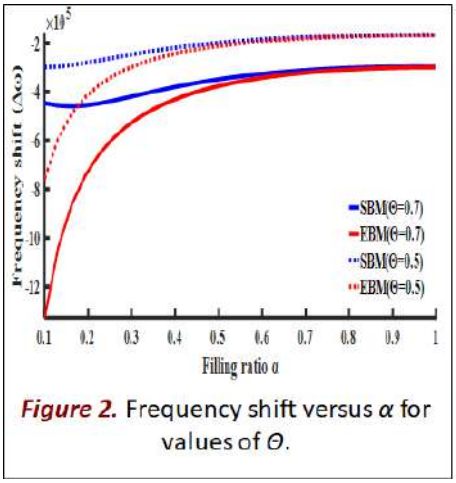


Figure 2. Frequency shift versus α for values of Θ.

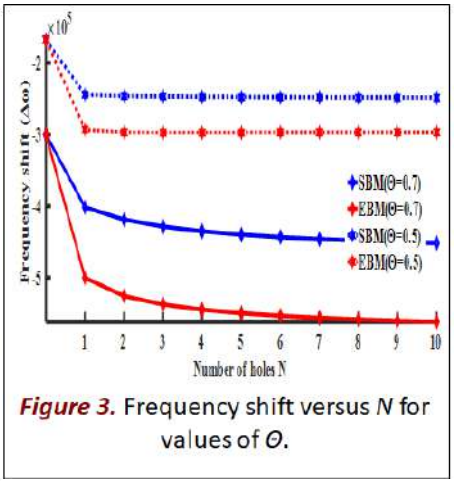


Figure 3. Frequency shift versus N for values of Θ.

4 Conclusion

The results indicate that the frequency shift observed in a system with holes is greater than that in an adatom-nanobeam system as a whole. This discrepancy arises from the shear effect, which leads to notable

differences between the changes predicted by the Euler Beam Model (EBM) and those determined by the Shear Beam Model (SBM) as the size of the nanobeam increases. These findings highlight the necessity of accounting for shear effects, establishing the SBM as the more suitable model for analyzing the adatom-nanobeam system.

To accurately predict dynamic vibrations, the non-local SBM should be preferred over the non-local EBM, which neglects shear stiffness effects. The presence of periodic square holes contributes to the softness of the adatom-nanobeam system, underscoring the advantages of using perforated nanostructures in the design of these systems. Additionally, the interplay between total bending and overall mass results in distinctive behaviors in response to variations in adatom density. Consequently, this study presents a physical framework that may prove beneficial in the development of microdevices for adatom sensing applications.

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Using advanced computational techniques to investigated the electronic, optical and thermodynamic properties of NaZrIrGe compound: DFT study

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Abstract

The NaZrIrGe quaternary compound exhibits intriguing electronic, thermodynamic, and optical characteristics, which have been thoroughly analyzed using first-principles calculations based on Density Functional Theory (DFT). Employing the full-potential linearized augmented plane wave (FPLAPW) method, this study utilizes the generalized gradient approximation (GGA) to gain insights into the compound's behaviour. The electronic structure reveals that NaZrIrGe possesses semiconductor properties. In addition to electronic properties, thermodynamic properties such as specific heat, entropy, isothermal bulk modulus, vibrational contribution and thermal expansion were examined, contributing valuable data for understanding the compound's response to temperature variations. These thermodynamic insights are crucial for evaluating its stability and performance in high-temperature applications. Furthermore, the optical properties including dielectric function, electrical conductivity, reflectivity, absorption coefficient, energy loss, and refractive index shed light on how NaZrIrGe interacts with electromagnetic radiation. These characteristics enhance the material's suitability for use in photovoltaic cells and optoelectronic devices. The combined understanding of its thermodynamic and optical behaviours reinforces NaZrIrGe's potential for advanced technological applications, particularly in energy and electronics sectors.

Keywords: Quaternary, DFT, Optoelectronic, Thermodynamic, Wien2k.

Main results

1- Structural properties

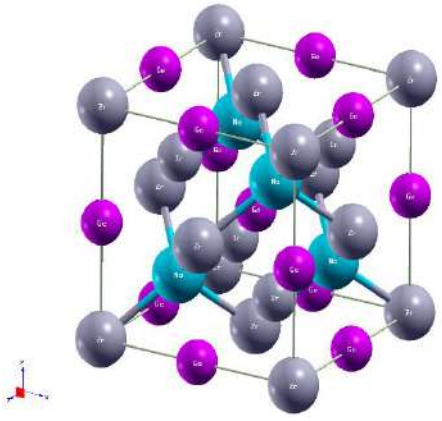


Fig. 1. *The structure of NaZrIrGe.*

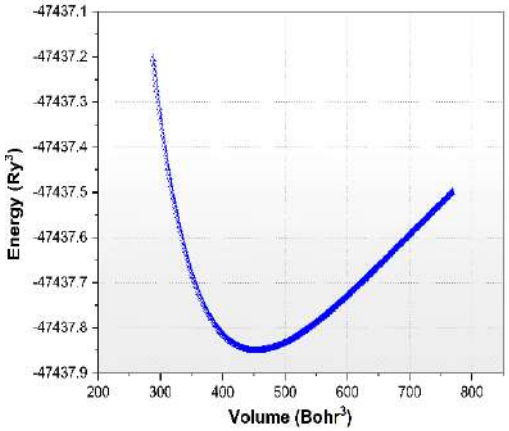


Fig. 2. *Total energy vs. volume for NaZrIrGe quaternary Heusler alloy.*

2- Electronic properties

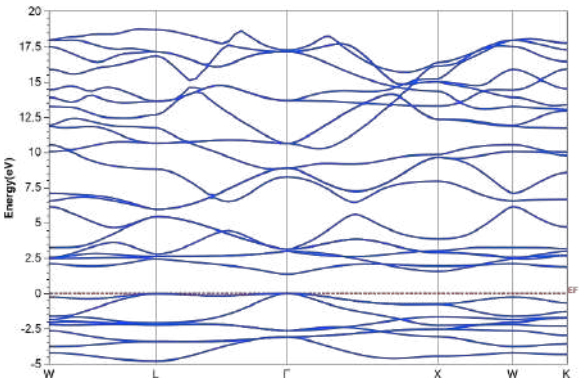


Figure 1The Band structure for NaZrIrGe compound.

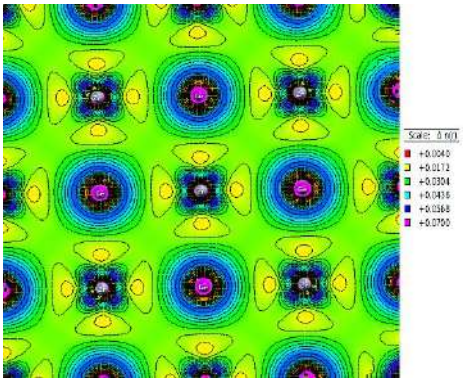


Fig. 4. The charge density of Zr and Ge atoms.

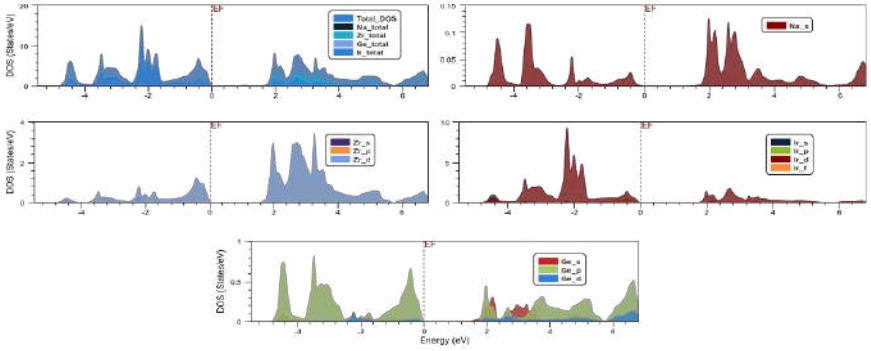


***Fig. 5**. PDOS and TDOS of NaZrIrGe.*

3- Thermodynamic and Optical properties

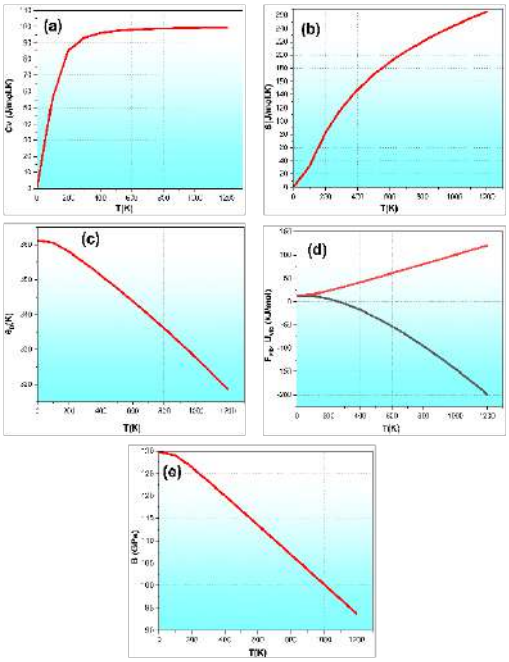


***Fig.6**. Thermodynamic properties.*

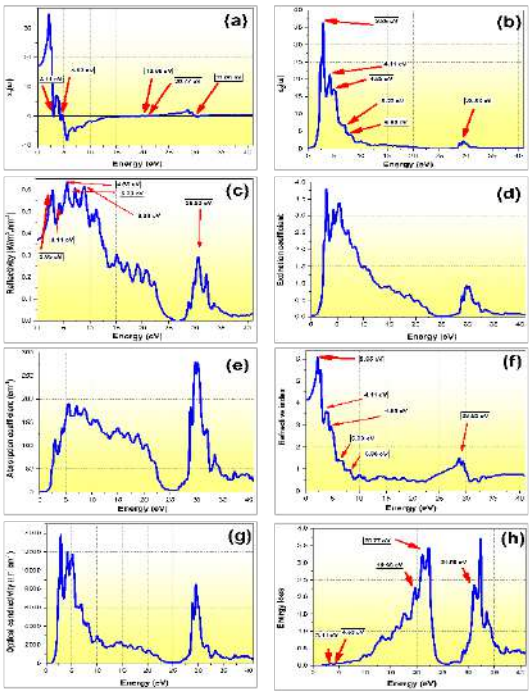


***Fig. 7**. Optical properties.*

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Catalytic activity of α-MnO_2 nanoparticles synthesized by hydrothermal method for the degradation of organic dyes

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Pollution of the environment and in particular pollution of water and air by organic compounds causes many health problems, hence the need to find suitable and effective solutions to fight against environmental pollution and preserve the lives of humans, animals and plants [1-2]. The present work is carried out in order to fabricate a catalyst material that is effective for the degradation of organic pollutants such as the Methylene Blue dye which is a widely used in textile industry [2,3].

The studied catalyst, α-MnO_2 nanoparticles, was synthesized using $KMnO_4$ and $MnSO_4.H_2O$ and deionized water as primary reagents introduced in sealed autoclave under following hydrothermal parameters (temperature 90°C during 24 hours and autogenously pressure)

The elaborated powder has been analyzed by different techniques such as the X-ray diffraction, Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, UV-Vis absorption and as well as scanning electron microscopy (SEM) to highlight their structural and optical characteristics. The analyses showed that the crystal structure of synthesized nanoparticles has the symmetry of the tetragonal space group I4/m of the α-MnO_2 phase and that the crystallites havea morphology of nanowires with a nanometricsquare cross section and a length of few microns. FT-IR and Raman spectroscopies confirmed the synthesis of the α-MnO_2 phase. The optical gap has been estimated at 3.30 eV. The evaluation of the degradation of Methylene Blue dye (MB) was conducted in the dark with the presence of α-MnO_2 crystallites. The catalytic degradation reached 67.10% for a reaction time of only 18 minutes. Thus, it allows us to notice the good efficiency of the synthesized α-MnO_2 catalyst.

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XRD Crystal Data Analysis, Hirshfeld surface analysis of 2,4,6-tris-(bromo-phenoxy-)-1,3,5-triazine (BrPOT) with 2,4,6-collidine.

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Abstract

In order to understand the behavior of the methyl radical (CH_3), a systematic study is carried out on benzene or cyclic products derived from highly symmetrical molecules substituted by methyl and halogen with biological interest. In our overall work, we determined on the one hand the crystal structure of 2,4,6-tris-(bromo-phenoxy-)-1,3,5-triazine (BrPOT) with 2,4,6-collidine which is resolved from X-ray diffraction from a single crystal at low temperature. The crystal structure of 2,4,6-tris-(bromo-phenoxy-)-1,3,5-triazine (BrPOT) with 2,4,6-collidine wich has been synthesized and determined from single crystal X-ray diffraction at low temperature (100K). This product crystallizes in the space group monoclinic P1 2_1 1. With two molecules per unit cell. The molecules are stacked by the repetition of collidine molecules along the crystallographic along the b-axis. The molecule is flat with deviations of ± 0.1A either side of the mean plane of the molecule.

Using the Crystal Explorer program, we analyzed the Hirshfeld surface, understand the crystal stacking and identified the intermolecular interactions that ensure cohesion in the crystal .A Hirshfeld surface calculation on the asymmetric unit of the collidine encaged in Br POT was carried out using Crystal Explorer 3.1 [1] to get a better understanding of the intermolecular interactions and their roles in the crystal cohesion and stabilization. The analysis of the two-dimensional finger print plots shed more light on the interaction's percentage and strength.

Key words: X-ray; Hirshfeld surface; biological interest, Single crystal, Modeling.

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Optimizing the Electrochemical Properties of ZnO Nanostructures through Eco-Friendly Synthesis Methods

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This work focuses on the biosynthesis of ZnO nanostructures using an extract from Tisane leaves, aimed at applications in water separation. The primary objective of this study is to explore the characteristics of ZnO samples synthesized through a green synthesis approach, with an emphasis on the use of Tisane extract. These samples were subsequently deposited onto copper substrates via pyrolysis, a method that facilitates the formation of nanostructures with enhanced properties.[1,2]

To evaluate the performance of these nanostructures, photoelectrochemical studies were conducted, specifically targeting their ability to produce hydrogen through water splitting. The results indicate effective electrochemical activity for oxidation and reduction reactions, revealing significantly improved anodic and cathodic peak currents as acquisition speed increases. These observations underscore the promising potential of ZnO nanostructures synthesized for electrochemical applications, particularly in a 0.1 M NaOH electrolyte solution.[3]

Furthermore, capacitance measurements and Mott-Schottky analyses were performed to examine in detail the interfaces between the semiconductor and the electrolyte. These analyses were executed by varying the applied constant current potential and frequency, allowing us to gain a deeper understanding of the electronic properties of the samples. Additionally, we determined carrier concentrations (N_D) and flat band potentials (V_{fb}) through Mott-Schottky analysis, providing essential insights into the structure and behavior of ZnO nanostructures in an electrochemical environment. These findings pave the way for further research into utilizing these nanostructures in water separation devices and other advanced electrochemical applications.[4,5]

Key word—Tisane leaf extract, electrochemical, green synthesis.

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Etude numérique de l'effet de la Stratégie de nids d'abeilles sur les pertes convectives dans la lame d'air d'un capteur solaire plan

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Dans cette étude, on a étudié numériquement à l'aide du logiciel Ansys Fluent l'effet de la stratégie de nids d'abeilles sur les pertes convectives dans la lame d'air situé entre l'absorbeur et la vitre d'un capteur solaire plan. Cette lame d'air et représentée par une cavité rectangulaire inclinée. Elle se compose d'une paroi inférieure (absorbeur) chauffée avec une densité de flux constante, des parois latérales isolantes (adiabatique) et une paroi supérieure qui représente la vitre. Cette dernière échange avec le milieu ambiant vers le haut par des flux convectifs et radiatifs (condition mixte). En ce qui concerne la stratégie étudiée, elle est représentée par des partitions attachées à la vitre avec une épaisseur constante et une distribution uniforme. Le but de ce travail est d'étudier l'effet du nombre et de la longueur des partitions sur les pertes convectives. Les résultats montrent que l'utilisation de cette stratégie peut conduire à la réduction des pertes convectives entre l'absorbeur et la vitre, et ce avec plus ou moins d'intensité selon la longueur et le nombre de partitions.

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Triple Differential Cross Section Calculations for the Positron Impact Ionization of Nitrogen Molecule in the Intermediate Energy Regime.

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Collisions between charged and neutral particles are fundamental in both atomic and particle physics. A key focus of research is electron-induced single ionization, or (e,2e), which helps to understand the dynamics of electrons and ions under external forces, a topic relevant to both atomic interactions and broader particle behavior. This phenomenon, involving the interaction between an incoming electron and a target atom or molecule, provides valuable insights into basic atomic and particle processes. Studying the ionization of nitrogen molecules is particularly significant, as nitrogen plays a crucial role in biological materials such as proteins and DNA.

In this study, we present theoretical triple differential cross sections (TDCS) for the ionization of nitrogen molecule (N_2) induced by positron impact, in the intermediate energy regime. Calculations are performed using three coulombian waves with variable charge model which was successfully applied for atoms [1] and extended here for N_2 molecule. The model, called M3CWZ for molecules, incorporates simultaneously the post-collisional interaction (PCI) and exchange effects. The TDCS results, obtained in asymmetric coplanar geometry, are presented as the sum contributions from the outer molecular orbitals $3\sigma_g$, $2\sigma_u$, $1\pi_u$, and the inner $2\sigma_g$ molecular orbital.

Our theoretical results are compared with the experimental data taken from De Lucio et al 2016 *Physical Review. A*. The comparison indicates an overall good agreement between our results and the experimental observations

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Predicting Perforation-Induced Frequency Shift in FGP Nanobeam Microsensors with Small scale Effects

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Abstract:

This study examines the vibration behavior of a simply supported Timoshenko sandwich nanobeam in the presence of surface effects. The nanobeam is composed of a functionally graded porous (FGP) material core that is positioned between two perforated layers with a regular square holes (RSH) network.

The nonlocal elasticity theory proposed by Eringen has been adopted to introduce small-scale effects. The Timoshenko beam equations are used to construct explicit formulations for the shear force and inertia moment, which include residual stress as an additive axial load.

Navier's type solution is used to solve these problems analytically. This study thoroughly examines the impact of the sandwich structure's geometric dimensions, perforation characteristics, nonlocal factors, and porosity coefficient. The results of this meticulous study have the potential to revolutionise the creation of more effective sensors and actuators.

Keywords: Timoshenko beam model, FGP sandwich nanobeam, Surface effects, Nonlocal elasticity theory, Regular square hole.

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Simulation of CIGTe-based Solar Cells Using SCAPS-1D with CdS as the Buffer Layerfor abstract

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This paper employs SCAPS-1D software to simulate a thin-film solar cell using the highly efficient Cu(InGa)Te2 (CIGTe). CIGTe proves to be an effective material for large-scale solar applications. Thin-film solar cells with the Mo/CIGTe/CdS/SnO2 configuration demonstrate improved performance. The enhancement is attributed to the impact of the window layer (SnO2) bandgap on key solar cell parameters, including short-circuit current density (JSC), open-circuit voltage (VOC), fill factor (FF), and overall CIGTe cell efficiency. Simulation results indicate a 21% increase in efficiency, with JSC, VOC, and FF values reaching 38 mA/cm², 0.67 V, and 83%, respectively.

Keywords

CIGTe,CdS, SnO2, SCAPS-1D

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Gate/Geant4 dosimetry using computational model

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Abstract

The radiation transport simulation by Monte Carlo techniques has become an important basic tool for dose calculations, and several program packages are currently available to deal with dosimetry problems in radiation protection and radiotherapy dosimetry.
In this work, GATE (version 9.1) has been used to derive absorbed fractions for the voxelized phantom computational model proposed by the International Commission on Radiological Protection (ICRP). Monoenergetic photons and electrons (from 50 keV to 1 MeV) were investigated to calculate the SAF (specific absorbed fraction) for the self-absorption and cross-irradiation. The particles were emitted from three source organs: kidneys, liver, and spleen. Furthermore, dosimetric parameters were calculated for three target regions in the body (kidneys, liver, and spleen).
The SAF values for self absorption largely depend on the radiation energy and organ mass and the SAF values for cross-irradiation are influenced by the relative placements of the source and target organs.

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Investigation of the Effects of SU(3) Color Representations on the Deconfinement Phase Transition from a Hadronic Gas to a Quark Gluon Plasma

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In the present work, we study the effects of SU(3) color representations on the deconfinement phase transition from a hadronic gas (HG) phase composed of massive pions to a quark gluon plasma (QGP) phase consisting of gluons, massless up and down quarks and massive strange quarks.

This study is carried out, using the phase coexistence model of the HG and QGP in a finite volume, as well as the group theoretical projection method, this in the calculation of some thermodynamical quantities characterizing the mixed hadronic gas-QGP, such as the order parameter, the energy density and the susceptibility.

The obtained analytical expressions of the physical quantities are calculated numerically, and the resulting data are plotted to obtain graphics of these quantities. Thus, we examine their behavior as a function of temperature at different volumes of the system and different SU(3) color representations for the QGP, namely the color singlet, the color octet, and the color 27-plet representation.

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Exploring the optical and photocatalytic properties of $Ca_{1-x}Mg_xTi_{1-y}Mn_yO_3$ powders synthesized by Sol-Gel method

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In order to improve the optical properties and photocatalytic performance of pure calcium titanate $CaTiO_3$ doped with Mg^{2+} (10 mol %) and co-doped with two ratios of Mn^{2+} (4 and 8 mol %). The resulting nanopowders synthesized by the Sol-Gel method were calcined at 900 °C for three hours. To comprehend more fully how the concentration of dopants affects the optical and structural characteristics of $CaTiO_3$ doped with Mg^{2+} (10 mol %) and two ratios of Mn^{2+} (4 and 8 mol %) perovskite nanostructures. Different characterization methods were used, such as powder X-ray diffraction (XRD), scanning electron mi-croscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), differ-ential scanning calorimetry (DSC-TG), Fourier transform infrared spec-troscopy (FTIR), Raman spectroscopy, and UV-visible spectroscopy. $CaTiO_3$ a perovskite-type oxide, has a wide bandgap (~3.7 eV), limiting its efficiency in photocatalytic applications that require UV light ab-sorption. However, the results show that the $CaTiO_3$ doped with Mg^{2+} (10 mol %) and co-doped with Mn^{2+} (10 mol %) exhibits significant photocatalytic activity, effectively degrading for the crystal violet dye under UV light irradiation

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Transport properties of Ca_3MN (M = P and As) antiperovskites using a new modified Beck-Johnson potential

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Lead halide perovskite materials have garnered significant attention due to their remarkable properties, including a suitable direct band gap, high optical absorption, long carrier diffusion length, and extended carrier lifetime. However, these materials face challenges such as degradation when exposed to water or air, and the toxicity of lead remains a significant environmental concern. Recent research has proposed antiperovskite semiconductors as potential substitutes for lead-based halide perovskites.

In this study, we investigate the electronic structure and transport properties of two calcium-based antiperovskites, Ca_3MN (M = P and As), using a newly modified Beck-Johnson potential. Both compounds are identified as wide band gap semiconductors, with their electronic structures predominantly influenced by the Ca *d*-orbitals and the *p*-orbitals of M and N. Our analysis reveals a net charge transfer from Ca to M and N atoms, consistent with the ionic configuration $(Ca^{+2})_3M^{-3}N^{-3}$. Furthermore, thermodynamic properties evaluated within the quasi-harmonic approximation show similarities between the two compounds, including low Debye temperatures. Notably, these materials exhibit high thermopower and soft phonon modes, indicating promising potential for thermoelectric applications.

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Impact of Copper Doping on the Ferromagnetic Properties of SrO

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This study examines the ferromagnetic and half-metallic properties of Cu-doped SrO at a concentration of 0.125. The growing importance of half-metallic materials in the field of spintronics has motivated this research, which aims to understand how copper doping influences the electronic and magnetic characteristics of SrO. Simulations were performed using density functional theory (DFT) [1] and the Wien2k code [2]. A supercell of 16 atoms was employed with the generalized gradient approximation (GGA-PBE) [3] to accurately model the system.

The results of our calculations show that the incorporation of copper into the crystal structure of SrO leads to an exceptionally high spin polarization, reaching almost 100%. This spin polarization is a key indicator of the half-metallic state of the material, where electrons with opposite spins exhibit distinct behaviors. Specifically, for one spin, Cu-doped SrO retains a metallic behavior, while for the other spin, it presents as a semiconductor with a wide band gap. This asymmetry in the electronic density of states is crucial for applications requiring spin manipulation, such as magnetic memories and spintronic transistors.

The electronic states of copper, particularly the d-t2g and d-eg states, play a significant role in inducing spin polarization and establishing the half-metallic state. These states contribute to the separation of the density of states, promoting the unique behavior of the material.

Furthermore, our analyses of the electronic structure reveal that copper doping significantly modifies the density of states (DOS) near the Fermi level. The DOS for one spin is strongly present at the Fermi level, while for the other spin, it is significantly reduced, creating the characteristic gap of a half-metal. This clear separation between spin states endows the material with its unique properties, making it particularly suitable for applications requiring spin-polarized conduction.

In conclusion, this study demonstrates that Cu-doped SrO possesses promising ferromagnetic and half-metallic properties, making this material an ideal candidate for advanced spintronic applications. The ability to modulate the electronic and magnetic properties of SrO through copper doping opens new avenues for the design of innovative spintronic technologies.

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The emission behavior of Tb^{3+} ion in the nanoscale solid solution $Y(V,P)O_4$

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Abstract:

Nanosized rare earth phosphovanadate phosphors (Y(P,V)O4:Tb3$^{+)}$ have been prepared using the sol-gel method.Luminescent powders with tetragonal structure and different vanadate concentrations were obtained for evaluation of their structural and spectroscopic properties.

The powders were characterized by scanning electron microscopy (SEM), X-ray diffractometry (XRD), Fourier Transform Infrared Spectroscopy (FT-IR), and photoluminescence spectroscopy, including room temperature steady-state and time-resolved photoluminescence spectroscopy (emission, excitation, and luminescence lifetimes).

The structural analysis reveals that the volume and crystallite size of the nanophosphors increase with increasing vanadium content, and their morphologies change from spherical, for low vanadium content, to rod-like for high content.

Blue and green PL emissions of Tb^{3+} and $(VO4)^{3-}$ were observed in $YP_{1-x}V_xO_4$. The solids exhibited a strong absorption band with a peak at 200 nm, attributed to the absorption of $(VO4)^{3-}$, and minor excitation bands corresponding to f→f transitions of Tb^{3+}. Two characteristic emission peaks were observed at 492 and 545 nm, attributed to $5D_4 \rightarrow 7Fj$ (j = 6, 5) transitions. The prominent green emission peak in photoluminescence ($5D_4 \rightarrow 7F_5$) was centered at 545 nm.

The structure and potential mechanism of light emission from phosphovanadate phosphors (Y(P,V)O4:Tb3^{+}) are discussed.

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CHARACTERIZATION OF MAGNESIUM DOPED SnO_2 THIN FILMS PREPARED BY CHEMICAL SOL-GEL METHOD

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Abstract: This study reports on the development and characterization of pure and magnesium-doped SnO2 thin films using a simple, low-cost chemical method known as sol-gel. The films prepared were deposited on glass slides using dip-coating technique. To studies the effect of doping on Tin oxide properties, various characterization methods were used, including XRD, Fourier transform infrared FTIR, MEB and Hall measurements. The XRD results show a tetragonal rutile structure, the grain size of the films obtained is nanometric, FTIR analysis shows that the prepared thin films contain O–Sn–O, Sn–OH, Mg–O, and OH–Mg–OH vibration modes, MEB studies showed an increase of grain sizes with increase in Mg concentration, this increase is resulted from coal, escence events with neighboring grains. The electrical studies through Hall measurements, reveal an increase in resistivity with rising Mg concentration, a transition from n-type to p-type conduction was observed at 9 wt% Mg doping.

Keywords: thin films, SnO2, sol-gel, dip-coating, Mg doping, electrical studies.

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Spray Pyrolysis-Derived CNTS for Photovoltaic Applications

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Abstract

Quaternary chalcogenide semiconductors are increasingly emerged as promising materials for thin film solar cells. Cu2NiSnS4 (CNTS) stands out among them as a particularly remarkable candidate, demonstrating potential as a next-generation absorber material in thin film solar cell technology. In This work, chemical spray pyrolysis route was employed to prepare Cu2NiSnS4 thin films on glass substrates, using DMF as a solvent under air ambient. The XRD results displayed that the as-deposited thin films are polycrystalline in nature with cubic structure and favorite orientation along the (111) from 300 to 410°C. The crystallite size was estimated by Scherrer's equation and was found to increase with increasing temperature up to 5 to12.00 nm. Examination of the film morphology indicates a granular and compact surface with structures with different particle sizes and shapes. The optical properties and band-gap values were estimated by UV-Vis absorption spectrum and the Tauc Equation. The optimised films exhibit semiconductor behaviour with a band-gap ranging from 1.1 eV to 1.7 eV and the Hall Effect measurement on the CNTS thin films indicated a p-type of conductivity for all films, making them ideal for use in the field of thin film solar cells.

Keywords: CNTS, thin films, chalcogenide material, spray pyrolysis, photovoltaic material, structural properties, optical properties

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Influence of solvent type on physical properties of sprayed Co3O4 thin films

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In this study, we investigate the influence of various solvents (distilled water, methanol, and ethanol) on the physical properties of Co_3O_4 thin films, elaborated via spray pyrolysis on glass substrates at 400°C with a deposition time of 10 min. Multiple characterization techniques were employed to analyze the film properties. XRD results revealed distinct structural differences among the films, showing that the film prepared with distilled water exhibited a polycrystalline structure with a preferred (311) orientation [1], whereas the films prepared with methanol and ethanol presented an amorphous structure. The film prepared with distilled water displayed a root-mean-square (RMS) roughness of 76.49 nm and a contact angle (CA) > 90°, indicating a hydrophobic nature, which is advantageous for absorber layers [1-2]. In contrast, the films prepared with methanol and ethanol demonstrated hydrophilic behavior, with CA < 90° and RMS values of 14.78 nm and 25.96 nm, respectively. UV-Visible spectroscopy analysis showed high transparency (> 80%) for the methanol and ethanol-prepared films, while the film prepared with distilled water had low transparency at 3%, signifying high absorbance with an optical band gap of 1.31 eV. Electrical characterization revealed low resistivity for the distilled water-prepared film, measured at 7.916×10^{-1} Ω.cm. These findings suggest that distilled water is the most effective solvent for producing Co_3O_4 thin films with properties favorable for solar cell applications, particularly as an absorber layer.

Keywords: Co_3O_4 thin films, Solvent type, XRD, AFM, Wettability characteristics.

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Growth factor parametrization

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Abstract

The growth rate of matter perturbations may differentiate between various general relativity dark energy models and between general relativity dark energy and modified gravity models in explaining cosmic acceleration. We suggest the analytical equation $f_r = \Omega_m^\gamma + \beta\Omega_r$ (where $\beta = \gamma - 2/3$) as an estimate for the growth factor f when radiation is considered. The growth factor is examined for dark energy models in the context of general relativity. The growth index γ assumes unique values for each model. The new analytical form f_r provides a superior approximation of f compared to Ω_m^γ.

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Structural study of Ni/MgO nanoparticles for biological application

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This work discusses Ni/MgO nanocmposites for use as antibacterial agents. The samples were prepared via impregnation (labeled NMI) followed by calcination at temperatures T ≥ 100°C (referred as NMC(T)). Various experimental techniques were used for their characterization: XRD, SEM, TEM, and HRTEM.

The structural study reveals the formation of magnesium hydroxide during the impregnation step, in addition to the formation of bimetallic Ni-Mg nanoparticles (Ni_2Mg, $NiMg_2$, $Mg_{6.33}$) with sizes ranging from 2 to 4 nm. These phases are present in both the impregnated sample (NMI) and in samples calcined at temperatures T ≤ 300°C. However, at temperatures T > 300°C, these phases disappear, giving rise to a new phase $NiMgO_2$.

MgO samples, Ni/MgO after impregnation (NMI) and Ni/MgO impregnated and calcined at 300°C and 400°C were tested as antibacterial agents against E. coli (G^-) and S. aureus (G^+). They exhibited toxicity towards both bacteria. This activity is attributed to $Mg(OH)_2$ on one hand, and on the other hand, to the synergistic effect of nickel and magnesium present in Ni-Mg and $NiMgO_2$ and at their size effect.

Key words : nanoparticles, Ni-Mg nanocomposites, antibacterial agents, XRD, SEM, TEM

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A first-principles calculation of structural, electronic, and thermoelectric properties of Hafnium-based compounds

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Abstract:

Thermoelectric materials have been studied for their potential to convert waste heat into electricity, aiming to reduce dependence on fossil fuels and conventional energy sources and the consequent carbon emissions. Solar energy is a highly effective renewable energy source, but its efficiency relies on the development of photovoltaic materials [1,2]. Recently, transition metal dichalcogenides (TMDCs) have received significant attention from researchers and scientists as a type of two-layered (2D) material due to their electronic, optical, mechanical, and thermal properties and their potential applications in electronic and solar energy-harvesting devices [2,3]. TMDCs are van der Waals multilayer semiconductors of type MX_2, with M representing a transition metal atom like Hf, Mo, or W and X representing a group-16 element like S, Se [2,4]. In this work, we focus on two simple TMDC materials, HfX_2 (X = S and Se). These materials exhibit high optical absorption in the visible spectrum and semiconducting behavior in both experimental and theoretical band gaps. Accordingly, HfX_2 (X = S, Se) can be further used as potential components in optical absorbers for next-generation solar cells [1].

Kohn–Sham density functional theory (DFT) with van der Waals forces proposed by Grimme [5] has been used to study the structural, electronic, and thermoelectric properties of HfX_2 (X=S or Se) in P–3m1 structures. All the first-principles calculations are performed using the ABINIT code and taking into account the van der Waals interaction by the empirical dispersion correction using the method of Grimme (DFT (PBE)-D3). Perdew-Burke-Ernzerhof (PBE) functional form of generalized gradient approximation (GGA) has been used for the exchange and correlation of electrons, and projector augmented wave (PAW). Furthermore, to explore the electronic structures and accurately predict the band gaps of HfS_2 and $HfSe_2$, TB-mBJ in ABINIT was employed from the Libxc package of exchange-correlation functions [6]. The temperature- and charge-carrier concentration-dependent thermoelectric properties were calculated using semi-classical Boltzmann transport theory and the constant scattering time approximation in the BoltzTraP2 code [7].

The compounds have an indirect bandgap ranging from 0.70 to 1.51 eV, and the band gap decreases as the chalcogen atomic size increases. The electrical conductivity (σ), Seebeck coefficient (S), and electronic thermal conductivity (k_e) of each material were measured depending on doping levels in the ab-plane (xx) and cross-plane (zz) directions.

Keywords: Transition metal dichalcogenides, van der Waals corrections, electronic properties, thermoelectric properties.

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Influence of Lewis number on double diffusive convection in an inclined porous square cavity subjected to a magnetic field

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This work presents a numerical investigation of double-diffusive convection within a 45°-tilted square porous cavity saturated with a Newtonian fluid and subjected to a uniform magnetic field. The cavity is subjected to horizontal temperature and vertical concentration gradients, inducing cross fluxes of heat and mass. The flow is modeled using the Darcy approximation, with a fixed thermal Rayleigh number of 150 and a buoyancy ratio (N) of 1.

This study focuses on the impact of the Lewis number (Le), representing the ratio of thermal to mass diffusivity, on the system dynamics. A parametric study is conducted by varying Le, exploring its effects on the temperature, concentration, and flow fields within the cavity.

The resulting convective patterns and their evolution with Le are analyzed. Furthermore, the influence of Le on heat and mass transfer rates is quantified through the Nusselt and Sherwood numbers, respectively. The interaction between the magnetic field, the inclination of the cavity, and the varying diffusivity ratio is examined. This research aims to provide a deeper understanding of the complex interplay between these parameters in double-diffusive convection within porous media.

The findings are relevant for a range of applications, including geothermal energy, contaminant transport, and material processing. The detailed results will be presented and discussed, highlighting the significant role of Le in controlling the overall system behavior.

Keywords: Double-diffusive convection, Porous media, Darcy model, Magnetic field, Inclined cavity, Lewis number, Nusselt number, Sherwood number.

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Van der Waals Black Hole in Deformed Space with Maximal Length

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Abstract

The cosmological particle horizon represents the maximum measurable distance in the Universe. The presence of this upper limit on observable length suggests a modification to the Heisenberg uncertainty principle. A modification of the Heisenberg uncertainty principle, aligned with the existence of a maximum observable length scale, is $\Delta X \Delta P = \frac{\hbar}{2} \frac{1}{1-\alpha(\Delta X)^2}$. In this paper, we investigate how this modification affects Van der Waals (VdW) black hole. To achieve this, we first calculated the modified lapse function and then derived the Hawking temperature and the components of the energy-momentum tensor based on Einstein's equations. Our results show that this formalism imposes an upper limit on the radius of the event horizon, and the corresponding stress-energy tensor obeys all three weak, strong, and dominant energy conditions.

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Numerical simulation of forced and mixed convection in a Taylor-Couette system subjected to differential heating

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The current study is a numerical simulation of the first instability appearance in a Taylor-Couette system subjected to radial differential heating. The working fluid confined in the annular space is assumed to be newtonian and incompressible, with thermo-dependent physical properties.

The main objective is to provide a better understanding of instability mechanisms by detecting the critical Reynolds numbers in both cases: horizontal ($\alpha = 0°$) and vertical position ($\alpha = 90°$) to optimize the best position for industrial heat systems involving rotational flows.

Using a second-order spatiotemporal discretization, the finite volume method is used to numerically solve the model of the conservation equations (mass, momentum and energy) and its associated boundary conditions. The approach takes buoyancy forces into account through the Boussinesq approximation, enabling the effect of differential heating on the formation of convective cells and flow regimes to be evaluated.

The obtained results demonstrate that the inclination angle α has no influence on the velocity field during forced convection. However, it affects the temperature field as well as the velocity field due to buoyancy effects. In addition, choosing the horizontal position is preferred from a thermal standpoint in order to obtain both dynamic and thermal stability.

Key words: *Instability, Finite Volume method, Taylor Vortex Flow, Differential heating, Mixed convection*

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Theoretical analysis of the structural, electronic and optical properties of ScXLu3 with (X = B or N)

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Abstract :

We have applied the pseudopotential linearized augmented plane wave (P-W) method to study the structural, elastic and electronic properties of the cubic antiperovskite-type ScXLu3, (X = B or N). The ground-state properties are in agreement with experimental data. We have employed the local density approximation (LDA) and the generalized gradient approximation (GGA) for the exchange and correlation potential[1]. The equilibrium lattice constants and the bulk modulus and its pressure derivative are calculated and compared with available experiment and theoretical results. we have also predicted the elastic constants, Young's modulus (E), Poisson ratio (υ), shear modulus (G). The contribution of the different bands was analyzed from total and partial density of states curves. We have estimated the sound velocities in the principal directions. Through the quasi-harmonic Debye model, in which the phononic effects are taken into account, the temperature and pressure effects on the lattice constant, bulk modulus, heat capacity and Debye temperature are performed[2].

Key words : Intermetallic compounds, Ab initio calculations, Elastic properties

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The number density of produced particles in a non-commutative curved space-time

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Our goal is to investigate the role of the external electric field and the non-commutative parameter in the emergence of particles from the vacuum of space-time. We have utilized the Bogoliubov transformation technique in order to calculate the number density of the produced particles in a non-commutative curved space-time.

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Dosimetric characteristics of 6 MV with and without flattening filter beams generated by the Varian TrueBeam linac used in radiotherapy treatments

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The use of flattening filter-free (FFF) radiation beams in external radiotherapy is arising as standard linear accelerators remove the flattening filter (FF), and research is focusing on the clinical benefits of this approach. Advanced treatment techniques have heightened interest in operating linear accelerators in FFF mode. [1].

This study aims to evaluate the dosimetric impact of FFF beam energy selection on treatment plan quality by presenting a systematic dosimetric comparison of plan quality between flattened (FF) and unflattened (FFF) photon beams at 6 MV from the Varian TrueBeam linear accelerator at the Hospital-University Center Dr. Abdesselam Benbadis in Constantine, Algeria [2]. The differences between the non-uniform dose distributions produced by removing the flattening filter (FF) and the uniform dose distributions were analyzed. These differences were evaluated in treatment plans for glioblastoma cancer patients using the plannification system “VARIAN Medical Systems Eclipse Version 18”.

The main advantage of the 6 MV FFF beam is its ability to reduce treatment time due to a higher dose rate, which improves accuracy by minimizing involuntary patient movements. However, the unflattened beam profile requires careful planning to avoid overdose in certain areas. In contrast, the traditional 6 MV beam offers better dose uniformity, which can be beneficial for treating tumors close to organs at risk.

The 6 MV FFF beam also reduces out-of-field dose, thereby minimizing exposure to healthy tissues, an important consideration in treating brain tumors like glioblastomas, where protecting surrounding tissues is crucial.

In summary, 6 MV FFF radiotherapy provides advantages in terms of speed and reduced out-of-field dose, while traditional 6 MV maintains better dose uniformity. The choice between these two options should be based on the specific characteristics of the patient, tumor location, and clinical treatment goals.

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Effect of the Bohm potential in a quantum dusty plasma.

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The classical hydrodynamic model provides a reliable description of the dust acoustic wave. Moreover, when the dimensions of the plasma system (the distance between particles) are comparable to the de Broglie wavelength, quantum effects (quantum diffraction and quantum statistical effects) become significant and cannot be ignored. We aim to extend the dust acoustic wave model to the quantum case by incorporating quantum effects. Starting from the same classical assumptions and introducing the term for quantum diffraction, while considering the weakly nonlinear regime, we have applied the reductive perturbation technique, based on stretched variables, to derive the K-dV type equation associated with a three-component plasma (electrons, ions, and dust grains).

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Influence of BSF Layer on the Performance of CIGS Based Photovoltaic Cells

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This work presents the remarkable performance of copper indium gallium selenide (CIGS)-based double heterojunction photovoltaic cells. To enhance all photovoltaic parameters, a novel solar cell structure (FTO/SnS2/CIGS/CuSbS2/Ni) is explored using SCAPS-1D simulation software. Key device parameters such as the thicknesses of the buffer, absorber, and back surface field (BSF) layers, as well as acceptor density, defect density, interface defect density, generation and recombination rates, operating temperature, current density, and quantum efficiency, have been investigated for solar cells with and without BSF layers. The inclusion of a BSF significantly improves performance parameters, including short-circuit current (Jsc), open-circuit voltage (Voc), fill factor (FF), and efficiency (η). Simulation results for a conventional CIGS cell (FTO/SnS2/CIGS/Ni) show an efficiency (η) of 29.12%, with a FF of 81.54%, Jsc of 43.27 mA/cm², and Voc of 0.82 V. In contrast, the introduction of the CuSbS2 BSF improves η to 34.67%, with a Voc of 4.21 V, Jsc of 43.81 mA/cm², and FF of 18.78%. These results demonstrate that the proposed CIGS-based double heterojunction solar cells offer a promising route for achieving higher efficiency compared to traditional designs.

Key terms: CIGS, Back surface field, solar cell, heterojunction

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Ne and Kr double ionization with interaction configuration

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Double ionization is a physical process in which an atom or molecule loses two electrons, leading to the creation of a doubly charged ion. This phenomenon typically occurs in high-energy interactions, such as intense laser pulses, electron impacts, or collisions with other particles. It represents a complex quantum mechanical event characterized by intricate electron-electron interactions and multi-body effects. Double ionization is significant across various scientific fields, including plasma physics, astrophysics, and high-energy physics. Configuration Interaction (CI) is a quantum mechanical method used to improve the accuracy of wave functions in multi-electron systems, particularly atoms and molecules. It addresses one of the major shortcomings of simpler methods, like the Hartree-Fock (HF) approximation, by accounting for electron correlation — the way electrons influence each other's motion due to their mutual Coulomb repulsion. For the Neon we have 15 functions and each represent a probability. The first work on neon has been done by Kada & al (1) and we'll explore more of it here:

J	*États*	m_l	m_s	$\phi_i^j(\vec{r}_1,\vec{r}_2)$
1	^3P	+1	+1	$\lvert np_1 np_0\rvert$
2	^3P	+1	-1	$\lvert n\bar{p}_1 n\bar{p}_0\rvert$
3	^3P	0	+1	$\lvert np_1 np_{-1}\rvert$
4	^3P	0	-1	$\lvert n\bar{p}_1 n\bar{p}_{-1}\rvert$
5	^3P	-1	+1	$\lvert np_{-1} np_0\rvert$
6	^3P	-1	-1	$\lvert n\bar{p}_{-1} n\bar{p}_0\rvert$
7	^3P	1	0	$^1/_{\sqrt{2}}(\lvert np_1 n\bar{p}_0\rvert + \lvert n\bar{p}_1 np_0\rvert)$
8	^3P	0	0	$^1/_{\sqrt{2}}(\lvert np_1 n\bar{p}_{-1}\rvert + \lvert n\bar{p}_1 np_{-1}\rvert)$
9	^3P	-1	0	$^1/_{\sqrt{2}}(\lvert np_{-1} n\bar{p}_0\rvert + \lvert n\bar{p}_{-1} np_0\rvert)$
10	^1D	2	0	$\lvert np_1 n\bar{p}_1\rvert$
11	^1D	-2	0	$\lvert np_{-1} n\bar{p}_{-1}\rvert$
12	^1D	+1	0	$^1/_{\sqrt{2}}(\lvert np_1 n\bar{p}_0\rvert - \lvert n\bar{p}_1 np_0\rvert)$
13	^1D	-1	0	$^1/_{\sqrt{2}}(\lvert np_0 n\bar{p}_{-1}\rvert - \lvert n\bar{p}_0 np_{-1}\rvert)$
14	^1D	0	0	$\frac{1}{\sqrt{6}}(\lvert np_1 n\bar{p}_{-1}\rvert - \lvert n\bar{p}_1 np_{-1}\rvert + 2\lvert np_0 n\bar{p}_0\rvert)$
15	^1S	0	0	$\frac{1}{\sqrt{3}}(-\lvert np_1 n\bar{p}_{-1}\rvert + \lvert n\bar{p}_1 np_{-1}\rvert + \lvert np_0 n\bar{p}_0\rvert)$

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Effet du dopage par Y^{3+} et Zr^{4+} sur les propriétés structurales et électrochimiques d'une électrode $SrFe_{1-x}M_xO_{3-\delta}$ pour pile à combustible (SOFC)

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Dans cette étude, nous avons élaboré par la méthode de réaction à l'état solide un matériau de cathode de structure pérovskite $Sr_{0.9}Zn_{0.1}Fe_{1-x}M_xO_{3-\delta}$ avec M=Y^{3+} et Zr^{4+} et x = 0, 0.05 et 0.10. Ce type d'électrode appelé la ferrite de strontium qui possède un état d'oxydation mixte de 3+ et 4+ dans le site B est un matériau intéressant dans la fabrication des piles à combustible à oxyde solide (SOFC).

L'objectif est d'étudier l'effet du dopage par l'yttrium (Y^{3+}) et le zirconium (Zr^{4+}) sur les propriétés structurales et électrochimiques de ces matériaux d'électrodes. Les échantillons ont été caractérisés par la diffraction de rayons X (DRX), le microscope électronique à balayage (MEB) et l'analyse par énergie dispersive (EDAX).

Les résultats obtenus par DRX ont confirmé sur la bonne cristallisation et la formation de la phase principale avec une proportion majoritaire. La fraction volumique la plus élevée de la phase principale est estimée au environ de 96 % pour un dopage de 0.05 en Y^{3+}. Cependant, une présence minoritaire de quelques phases secondaires est détectée surtout dans l'échantillon dopé par 0,1 de Zr^{4+}. L'affinement des paramètres de maille et les facteurs d'agréments des échantillons est réalisé dans le système tétragonale de groupes d'espaces I4/m mm, de même la taille moyenne des cristallites calculée par la méthode de Deby Scherrer est d'ordre nanométrique (~22nm).

Les études électrochimiques sont réalisées à la température ambiante dans un milieu alcalin de NaOH à 0.5M en utilisant les techniques de spectroscopie d'impédance (SIE), voltampérométrie cyclique (CV) et l'application du model de Mott Schottky. Les plots de Mott Schottky des échantillons $Sr_{0.9}Zn_{0.1}FeO_{3-\delta}$ et $Sr_{0.9}Zn_{0.1}Fe_{0.9}Zr_{0.1}O_{3-\delta}$ ont révélé sur un comportement semi-conducteur de type P-P avec des valeurs de bande plate de +0.65 V /SCE et +0.54 V/SCE, respectivement. Les voltampérogrammes cyclique et les valeurs de bande plate ont montré que le dopage par Zr a amélioré le pouvoir réducteur de notre matériau d'électrode. Les diagrammes de Nyquist des électrocatalyseurs attestent sur la présence des demi-cercles dans les trois domaines de fréquences HF, MF et BF.

Mots-clés : Cathode (SOFC), Dopage, Structure et microstructure, Mesures électrochimiques.

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Analytic Solutions of a Generalization of the Three-Body Problem of Calogero-Type Using SUSY-QM and SGA Approaches

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We display the algebraic derivation of the eigenvalues via both the well-known method of SUperSYmmetric Quantum Mechanics (SUSY-QM) and an independent group theoretic method, namely the Spectrum Generating Algebra (SGA), for a non-relativistic Hamiltonian describing a three-body problem of a bound quantum system.

This system is consisted of three light particles moving on real line confined within a Coulomb-like field and interacting with each other via both translationally invariant two particles interactions of Calogero type and additional non-translationally invariant three-body potentials, as well as a translationally invariant three-body potentials.

We expose the equivalence of the two methods by developing an algebraic framework through the Shape Invariance (SI) property.

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Exploring the physical properties of some B2 rare-earth intermetallic compounds and the MnV intermetallic: a comparative study.

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In this work, the pseudo-potential method based on the density functional theory (DFT) implemented in the VASP code was used to examine the physical properties of the Re-Ag (Re=Y, La, Ce, and Dy) and Re-Cu Re=Y, Dy, Ho, and Er) members of a class of fully ordered stoichiometric intermetallics compared with MnV ductile intermetallic, a candidate to replace these rare earth intermetallics, which crystallized in the CsCl-type B2 phase.

The B2 rare earth intermetallic compounds have been found to possess significant polycrystalline ductility at room temperature[1-3]. The calculated ground state properties such as lattice constants, bulk modulus, and elastic constants agree well with the available data. The ductility or brittleness of these materials is predicted for ErCu and HoCu compounds. The mechanical and Debye temperatures are expected from the calculated values of elastic constants.

The analysis of the density of states (DOS) [4] explains the contribution of atomic orbital characters to the energy bands. Furthermore, the chemical bonding of some the studies compounds was evaluated using the topological analysis method, which is based on the theory of atoms in molecules. Based on the obtained results, it can be concluded that these B2-type intermetallic compounds have very interesting mechanical and thermal properties for structural applications.

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Experimental study of temperature changes in the collector and absorber of a solar chimney

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With the increase in population and the advancement of living standards, energy has become more and more necessary. The shift towards clean (renewable) energies can be attributed to their clean nature, limitless supply, and growing competitiveness [1,2].

The purpose of the current study is to conduct an experimental investigation into the effects of ambient temperature and solar radiation on the mean temperature of the absorber and collector of the solar chimney. To achieve this goal, a solar chimney prototype with a collector diameter of 0.79 m, a collector height of 0.105 m, a chimney diameter of 0.075 m, and a chimney height of 1.39 m was constructed at M'sila University. The experiments were conducted in a arid climate at the Biskra University. The results show that the mean absorber temperature was higher than the mean collector temperature. The absorber and collector temperatures are correlated by a polynomial law. The ambient temperature and solar radiation have a significant impact on the mean temperature changes of the absorber and collector. Mathematical models that depict how the mean collector and mean absorber temperatures change with respect to solar radiation and ambient temperature have been proposed.

KEYWORDS: Solar chimney, Absorber temperature, Collector temperature, Solar radiation, Ambient temperature, Mathematical models.

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Capacitance-Voltage Characteristics of As-Deposited and Annealed NiO/Ga_2O_3 Heterojunction Diodes

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Abstract: With the rising demand for ultra-wide bandgap (WBG) semiconductors in power electronics and optoelectronics, Ga_2O_3 has emerged as a promising candidate due to its high dielectric strength, stability, and cost-effectiveness. NiO/Ga_2O_3 heterojunction diodes (HJDs) combine the benefits of Ga_2O_3 ultra-wide bandgap with NiO p-type characteristics, creating a diode suitable for high-voltage and high-temperature applications. This study provides a detailed examination of the temperature-dependent capacitance-voltage (C-V) characteristics of NiO/Ga_2O_3 HJDs, focusing on effective doping density (N_{eff}) and potential barrier (V_B). To enhance modelling accuracy, the study employs swarm optimization (PSO) algorithm to extract the diode C-V parameters. PSO demonstrated strong performance across a wide range of temperatures, as evidenced by its low root mean square error (RMSE), confirming its potential for optimizing complex semiconductor parameters. The analysis reveals an unexpected decrease in effective doping density (N_{eff}) with rising temperatures, which is attributed to electron traps identified through deep level transient spectroscopy (DLTS) and Laplace-DLTS. These findings lay a foundation for optimizing Ga_2O_3-based heterojunction devices for power electronics, suggesting that advanced AI techniques, such as PSO, could significantly aid in precise parameter extraction and device design.

Keywords: NiO/Ga_2O_3 heterojunction, capacitance-voltage characteristics, deep level transient spectroscopy, particle swarm optimization.

Structure

Figure 1. shows a cross section of NiO/Ga_2O_3 heterojunction diode.

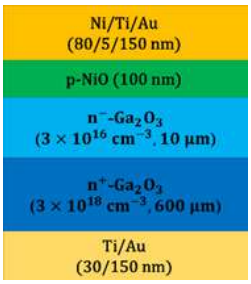


Figure 1. Schematic cross section of NiO/Ga_2O_3 HJD.

Analysis

Capacitance-voltage characteristics were measured at temperatures ranging from 160 K to 440 K at a frequency of 1 MHz for as-deposited and annealed samples. N_{eff} and V_B were extracted from 1/C2 plot using the following well-known approach [1]:

$$\frac{A^2}{C^2} \approx \frac{2(V_B - V)}{q\varepsilon_D N_D} \tag{2}$$

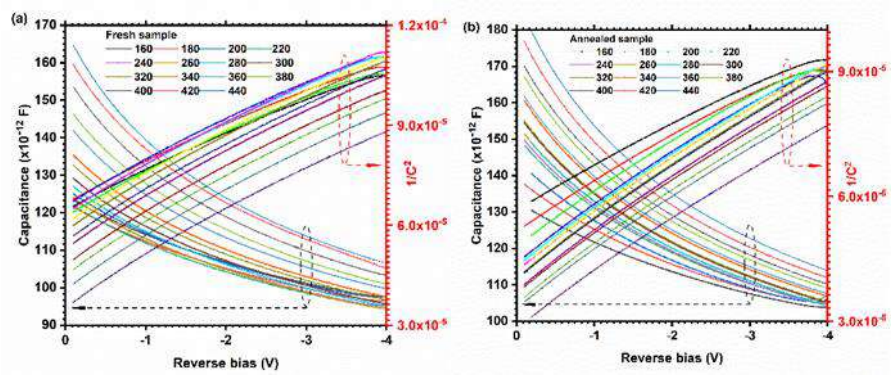


Figure 2: The reverse bias NiO/β-Ga2O3 HJD capacitance-voltage characteristics together with the corresponding 1/C2-voltage measured at a frequency of 1 MHz over a temperature range of 160-440 K for the as-deposited (a) and annealed (b) samples [2].

Results

N_{eff} and potential V_B and their evolution with temperature are presented in Figure 3:

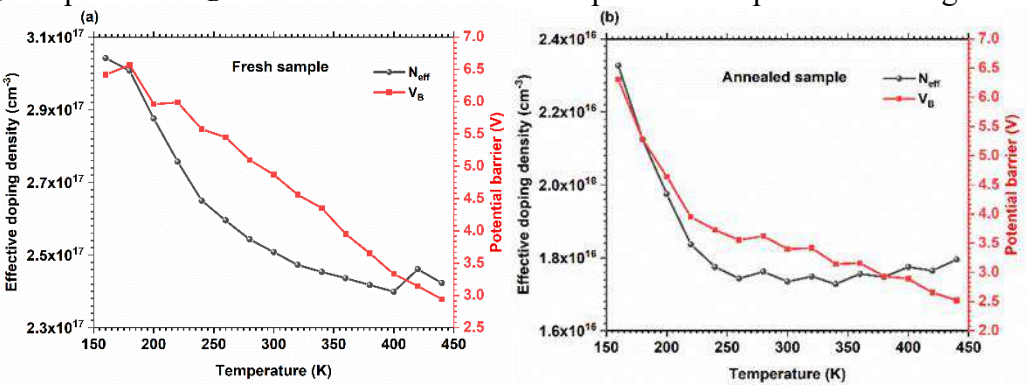


Figure 3: Effective doping density (N_{eff}) and potential barrier (V_B) at temperatures ranging from 160 K to 440 K for as-deposited (fresh) (a) and annealed (b) samples.

Table 1: The root mean square error of PSO algorithm for the as-deposited and annealed samples at different temperatures.

Temperature	As-deposited	Annealed
160	4.650×10^{-13}	4.919×10^{-13}
300	5.899×10^{-13}	7.280×10^{-13}
440	1.076×10^{-12}	8.408×10^{-13}

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Role of the Solvent in Enhancing the Magnetization of Iron Oxide Nanoparticles Synthesized via Co-precipitation.

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The development of nanosized particles is a promising research topic. Such particle sizes impart unique and novel physical and chemical properties to the material. Metal oxides, particularly iron oxides, exemplify the advantages of reducing particle size to achieve new or enhanced properties.

Iron oxides have been selected for their rich electronic and, most importantly, magnetic properties. Fe_3O_4 powders have gained considerable attention due to their potential applications in spintronics. This material has been predicted to exhibit half-metallic behavior, with a Curie temperature high enough to enable its use at room temperature in magnetoresistive devices.

In this context, we present here a low-cost co-precipitation method as a liquid-phase synthesis approach, using iron chloride as a precursor and various solvents (ethanol and HCl) for the synthesis of iron oxide nanoparticles. Lowering the pH induced the formation of a single phase corresponding to magnetite, with a superparamagnetic nature. The nanoparticles obtained from optimized synthesis conditions were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), and Raman spectroscopy.

The magnetic properties of the samples were analyzed using a vibrating sample magnetometer (VSM). The XRD results confirmed the formation of a pure phase (Fe_3O_4). High saturation magnetizations of 27.3 emu/g and 29.0 emu/g were achieved for nanoparticles synthesized with hydrogen chloride or hydrochloric acid (HCl). The increase in saturation magnetization is correlated with a reduction in magnetocrystalline anisotropy.

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Comparison of various thickness of nickel sulfide thin films prepared by spin coating method

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Sulfides thin films have become integral in various technical industries, notably in photovoltaic and electrical energy applications. Nickel sulfide thin films were prepared using sol-gel spin coating (SC) method on substrates of the glass at a temperature of 300°k. Current research has commenced synthesizing nickel nitrate hexahydrate and thiourea as a source of nickel and sulfur respectively. The coating process was repeated 04, 06,08, 10 layers times to obtain a good nickel sulfide thin film. The annealed sample was analyzed by X-ray Grazing incidence diffraction (GID) with a Bruker D8 Advance diffractometer using Cu Kα1 radiation at 40 kV and 40 mA (1600 W), Fourier transmission infrared (FTIR), Scanning electron microscopy (SEM) with energy dispersive X-Ray spectrometer (EDX), four-point probe measurement and atomic force microscope (AFM). The characterization methods indicate remarkable changes in the structural, morphological and electrical properties of nickel sulfide thin films. All films exhibited a cubic structure with nanoparticles, the surface of thin films is continuous and uniform with higher conductivity. The FTIR spectra belong to the NiS_2. EDX confirmed the formation of NiS_2. The composition confirmed by EDX analysis showed the presence of nickel and sulfur over the entire surface of the thin films with similar values in the three samples.

Keywords: Nickel Sulfide; thin films; Nanostructure; Spin coating; Thickness

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Enhanced photoelectrochemical Performance of Cu_2O/TiO_2 Nanowires

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The Cu_2O nanoparticles/TiO_2 nanowires (NWs) hybrid structure combines the advantages of the high surface area of TiO_2 NWs and absorption in the ultraviolet-visible light range. This structure can be used for various applications such as photoelectrochemical water splitting and photocatalysis. Cu_2O nanoparticles (NPs) were deposited onto TiO_2 NWs prepared by hydrothermal synthesis on Ti sheets using an immersion method. The obtained materials were characterized using XRD, SEM, UV/Vis diffuse reflectance, Raman, and XPS. The results revealed the formation of rutile and anatase crystalline phases together with Cu_2O, which shifts the absorption threshold of TiO_2 NWs into the visible spectrum range and enhances the photocurrent compared to bare TiO_2 NWs. Impedance measurements showed an increase in series resistance and a decrease in charge transfer resistance when decorated with Cu_2O. The photocurrent may depend not only on the Cu_2O coating but also on the anatase to rutile phase ratio in the TiO_2 NWs.

Keywords: Cu_2O NPs/TiO_2 nanowires, hydrothermal method, photoelectrochemical water splitting.

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Scale invariant triplet extension of the standard model with custodial symmetry

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In this work, we construct a scale-invariant extension of the Georgi-Machacek model [1], which is a triplet extension of the Standard Model (SM) that preserves custodial symmetries. Scale-invariant extensions of the SM were first introduced in the seminal paper by Coleman and Weinberg [2] and later extended to more complicated models involving multiple scalar fields by Gildner and Weinberg [3]. In our model, after writing the scalar potential of the extended Georgi-Machacek model, we use the Gildner method to find a minimum ground state called a flat direction. We then compute the one-loop effective potential and derive the mass spectrum of the model. Next, we apply theoretical constraints such as vacuum stability and perturbative unitarity, in addition to experimental constraints from the electroweak oblique parameter S and Higgs invisible decays, to study the parameter space of the model. We find that there is a region in the parameter space of the model compatible with all constraints.
Keywords: Scale invariance; Georgi Machacek model; mass generation

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The First International Congress on Recent Advances in Mathematical, Physical and Chemical Sciences (1st-ICRAMPCS 2024) December 15-17, 2024. Constantine. Algeria

Structural study of silver oxide nanoparticles fixed on TiO_2

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Due to their interesting chemical and physical properties, silver oxide has drawn attention for various scientific applications, particularly, in photocatalysis and biomedical fields [1].

The present work deals with the structural study of silver oxide nanoparticles fixed on titanium oxide. The sample is synthesised via a facile chemical reaction, at room temperature. In the beginning, the adsorption of silver ions on TiO_2 in wet conditions is optimized, where silver nitrate ($AgNO_3$) is used as silver source. After that, the sample is drying at 80°C for 24 hours. Finally, the sample is ready to be characterized by the X ray diffraction (XRD), Transmission Electron Microscopy (TEM) and Fourier Transform Infrared Spectroscopy (FTIR).

XRD pattern present the features of monoclinic silver oxide and anatase titanium oxide (TiO2) phases [2, 3]. These results are in good agreement with TEM results, which indicate uniform distribution of spherical shaped silver oxide nanoparticles fixed on titanium oxide surface with an average size estimated 5 to 20 nm. FTIR spectroscopy allowed the observation of vibration band at 618 cm^{-1} corresponding to the metal-oxygen banding vibration of Ag-O [4].

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Synthesis, Characterization, and Catalytic Activity of Copper(II) Oxide (CuO) Nanoparticles

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Nanotechnology has revolutionized solid-state chemistry by enhancing surface area as particle size decreases, which has made semiconductor nanoparticles (NPs) highly attractive for a wide range of applications, including photocatalysis, optoelectronics, solar cells and water purification [1]. Among these materials, transition metal oxides like copper (II) oxide (CuO) play a pivotal role in fields such as magnetic storage, solar energy conversion, electronics, and catalysis [2]. Due to its narrow band gap within the visible light spectrum, CuO is particularly suitable for photoconductive and photothermal applications [3]. The properties of these NPs are heavily influenced by the synthesis method and process parameters. These parameters affect the morphology, growth and yield of the NPsacross various synthesis techniques. In particular, hydrothermal synthesis has proven effective for CuO NPs production.

In this study, to assess the catalytic performances of CuO NPs in degrading methylene blue dye (MB), pure CuO NPs were synthesized using $CuSO_4 \cdot 5H_2O$ and NaOH as precursors applying the hydrothermal method. X-ray diffraction (XRD) analysis confirmed that the CuO NPs exhibited a monoclinic structure (C2/c) with crystallite sizes ranging from 9.64 to 26.08 nm. Infrared and Raman spectroscopy validated the successful synthesis, revealing Cu–O bond vibrations characteristic of CuO compound. Scanning electron microscopy (SEM) micrographs displayed an irregular platelet-like morphology with a surface area of 0.061 µm² and nanometric thickness. Brunauer-Emmett-Teller (BET) analysis indicated a specific surface area of 9.04 m²/g, suggesting potential for catalytic activity. The catalytic degradation of MB in aqueous solution by pure CuO NPs was initially limited to 19.77% after 60 minutes. However, when H_2O_2 was introduced, the degradation efficiency was significantly enhanced, reaching 100% within 40 minutes. Additionally, the synthesized CuO NPs demonstrated notable catalytic stability, retaining efficiency during recycling tests. Even after the second recycling test, the degradation rate of MB remained high, indicating the robustness and reusability of the synthesized CuO NPs. These findings highlight the promise of CuO NPs, especially with their platelet-like structure, for high catalytic activity in the degradation of organic dyes such as MB. Their stability and performance during recycling further emphasize their potential in environmental applications.

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Numerical Comparative Study of the Pipes Orientation in Photothermal Panel Subjected to a Non-Uniform Heat Flux

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The present work is a numerical simulation which concerns the effect of the pipes orientation on the heat transferred to fluid in photothermal panel. Tow configuration are studied: in the first one, the pipes in the panel are oriented horizontally but in the second configuration, the orientation is in the vertical direction. The panel is inclined from the horizon, the studied inclination angles are: α=30° and 60°.

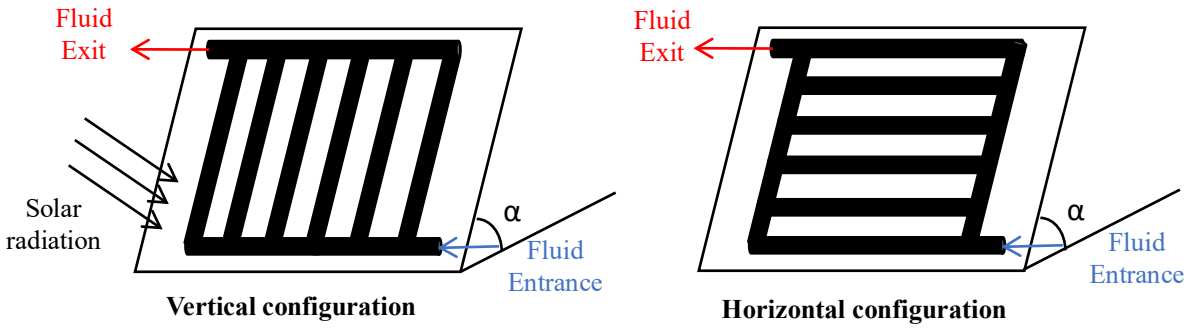


Figure 1: Configuration of the problem

The working fluid is considered Newtonian and incompressible with thermo-dependent physical properties. The model equations of continuity, momenta and energy are numerically solved by the finite volume method with a second order spatiotemporal discretization. The Prandtl, the Reynolds and the Grashof numbers are fixed at 8.0, 500 and 10^5 respectively.

The obtained results show that the dynamic and thermal fields for horizontal configuration are qualitatively and quantitatively different from those of vertical configuration. The heat transfer is quantified by the local and average Nusselt numbers.

The obtained results also show that the average Nusselt number at the tubes interface increases with the decrease of the inclination panel angle and the heat transferred to the fluid in horizontal configuration is greater than that in vertical configuration.

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Geodesic equation of test particles around a non-commutative Reissner-Nordström black hole: Analytical solutions in the gauge theory of gravity

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Abstract

In this study, we construct the deformed metric $\hat{g}_{\mu\nu}(r,\Theta)$ for the Reissner-Nordström black hole using the Seiberg-Witten maps [1], where the deformed Einstein gravity is considered in a non-commutative (NC) spacetime framework [2]. The resulting NC corrections to the metric allow us to investigate the orbital dynamics of a neutral massive test particle. The geodesic equation for this particle is derived up to the second-order correction in the NC parameter Θ, and an analytical solution is obtained using the method of successive approximations [3]. Furthermore, we analyze the impact of this modified geometry on the orbital motion of the neutral massive test particle in the RN spacetime.

Keywords: Geodesic equation; Non-commutative gauge theory; Reissner-Nordström black hole, Gauge theory of gravity

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Second Harmonic Generation with Quasi Phase Matching in PPGaN

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Nonlinear optics has recently been enhanced by the introduction of structures with periodically modulated nonlinear coefficients. The development of structures for periodically-poled in one or two dimensions allows very efficient quasi-phase matching (QPM) technique.

Efficient frequency conversion is achieved by using a high value of nonlinear coefficient with a verified phase matching condition. In some materials, such as III-V semiconductors, achieving phase matching through birefringence is challenging due to insufficient compensation for the dispersion in the indices of refraction.

For the many demonstrations of frequency conversion in GaN, the success of GaN as an efficient frequency converter will need the ability to fabricate periodically-poled GaN or PPGaN. These materials are known for large nonlinear susceptibility values and appear promising for achieving efficient nonlinear interactions.

Therefore, our study is based on the demonstration of second harmonic generation (SHG) in periodically-poled GaN (PPGaN) by first-order quasi-phase matching. This study is based on theoretical analysis to identify the crucial characteristics that must be taken into account to achieve effective frequency doubling.

The different parameters of structure and more particularly the power of incidence of the beam act on the phase-matching conditions to generate any wavelength contained in the range of transparency of the material. We utilised PPGaN with period 17um with a 50% duty cycle so that the PPGaN would produce SHG.

We observed about 12.9% W^{-1} cm^{-2} of normalized conversion efficiency ($n_{nor}\left[\frac{p_{2\omega}}{p_{\omega}^2 L^2}\right]$) from a fundamental input laser wavelength of 1659 nm. The capacity for nonlinear wavelength conversion, coupled with GaN's wide transparency range, paves the way for its use in nonlinear optical devices for telecommunications.

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mediated semi-quantum cryptography

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Abstract

Cryptography is the science and art of secret communication. With the use of a secret key, two parties can exchange messages in a format that is unreadable to an unauthorized third party. However, the algorithms currently in use are facing serious threats with the advancement of technology, especially with the emergence of quantum computers. To counter this issue, quantum cryptography offers a promising alternative. In this case, the security of communication is based on the laws of quantum physics rather than the mathematical complexity of the algorithms used.

The first quantum cryptographic protocol, known as BB84 [1], was developed by Bennett and Brassard in 1984. It allows two parties to exchange a secret key over a quantum channel using single qubits. Since then, many other protocols have been created [4, 8, 12, 7], utilizing different quantum resources such as entangled states and multi-level systems. Several of these protocols have been proven to be unconditionally secure [10, 9], meaning that their security is guaranteed regardless of an adversary's computational power. However, these proofs assume ideal conditions. In practical implementations, we must deal with noise and imperfect devices. Additionally, the quantum technology required to implement these protocols is costly and still in its early stages [3], making large-scale implementation of quantum cryptography a distant goal.

In response, Boyer et al. [2] introduced the concept of "semi-quantum cryptography" in 2007. This approach enables secure communication between a fully quantum-capable party and a classical user with limited quantum capabilities. This concept was initially proposed to address the question: "How much quantum is needed in a protocol or system to gain an advantage over its classical counterpart?" [5]. This question is crucial both theoretically and experimentally because by reducing the quantum overhead to what current technology allows, while still ensuring strong security, we can create implementable protocols that offer the same level of security as fully quantum ones.

In our work, we explore a recently introduced model of the semi-quantum environment known as the mediated model [6]. In this model, the parties involved are all classical and aim to establish a secret key securely, with the assistance of an adversarial quantum user who may attempt any possible attack to steal the secret. This model offers several key advantages over the traditional semi-quantum model [5]. First, all parties have the same limited quantum capabilities, significantly

reducing the quantum resources required. Second, any party can choose to share its secret key, enhancing the practicality of the protocols. Lastly, the model addresses the critical question of how classical parties can defend themselves against a quantum user participating in the protocol. In this study, we present the different challenges and needs encountered in semi-quantum cryptography and demonstrate how our work [11] in the mediated model addresses these problems. Additionally, we highlight potential research directions for future studies.

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NONCOMMUTATIVE SUPERSYMMETRIC THEORY

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Abstract

The objectif of this work is to treat the deformation of noncommutative U*(1) gauge supersymmetric theory N=1 in two dimensions: the noncommutative Poincaré superalgebra, and the noncommutative relations that the operators of this algebra verify, then we will give an overview of the noncommutative superspace in which this theory is constructed. Subsequently we will move on to writing this theory in terms of superfields. At the end, we will examine some noncommutative supersymmetric theoretical models.

Keywords: Gauge theory, Supersymmetry, Poincaré superalgebra, Noncommutative field theory.

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Noncommutative Schwarzschild Geodesics and Periastron advance of planet orbit

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Abstract

In this study, we construct a non-commutative gauge theory of the modified structure of the gravitational field using the Seiberg-Witten map and the general tetrad fields of the curved space-time to show that the non-commutative geometry removes the singularity at the origin of the Schwarzschild black hole, thus obtaining a non-singular Schwarzschild black hole. The geodetic structure of this black hole presents new types of motion next to the event horizon within stable orbits that are not allowed by the ordinary curved spacetime. The noncommutative periastron advance of the Mercury orbit is obtained.

Keywords: Non-commutative gauge theory, Schwarzschild black hole, Geodesic equation.

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Heat current correlations in a quantum Hall regime.

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Abstract
In this study, we investigate the heat current-current correlation between two edge states coupled by a constriction in a fractional quantum Hall regime. We choose the value $\nu = 1/3$ of the filling factor [1]. This value allows us to use a mapping between our system and an interacting Tomonaga-Lüttinger liquid with impurity located at $x = 0$ [2, 3, 4]. Chosing the value $\nu = 3$ imposes the interaction constant in the Tomonaga-Lüttinger liquid to take the value $K = 1/2$. This value allows us to use the refermionization method [5]. Using the wave function solution of the refermionized Hamiltonian [6], we compute the heat current and the finite frequency heat auto-correlations and cross-correlations. The graphical representations shows an asymetric behavior corresponding to different contributions to the noise between absorption and emission frequencies. Several limit cases are tested, such as the zero frequency $\omega = 0$, or the perfect transmission $\mathcal{T} = 1$.

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Crystal structure and Hirshfeld surface analysis of N-((4-chlorophenyl) (2-hydroxynaphtalene-1-yl) methyl) acetamide

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We are going to present in this abstract the crystallographic characteristics and the Hirshfeld properties of the synthesised N-((4-chlorophenyl) (2-hydroxynaphtalene-1-yl) methyl) acetamide (CHMA).

This compound known as a derivative of 1-amidoalkyl-2-naphthol, this family of compounds has an important role in the manufacturing of medicinal and pharmaceutical products, hence comes our great interest on these compounds.

After Synthesis of our title compound, CHMA was the subject of a crystal structural determination at room temperature.

X-ray diffraction has been established using a diffractometer Bruker-AXS APEX2 [1]. The structural resolution was carried out by direct methods using the chain program WinGX [2], SIR92 [3]. The refinement of the positions and movement parameters was made using the SHELXL 2018 program [4].

X-ray diffraction analysis showed that the CHMA crystallizes in the space group P2 1 /n of the monoclinic crystal system with four (4) molecules per unit cell.

In the crystal, adjacent molecules are interconnected by hydrogen bonds O-H···O and C-H…Cl to form a one-dimensional chains following [010] direction. These chains are attached together by the short contact C-H…C to create a two-dimensional shape following the [001] direction. The superposition of the two-dimensional layers, following the [100] direction, creates the shape three-dimensional crystal (fig. 1.B).

The cohesion of the crystal structure is also ensured by π-π interactions type (fig. 1.A).

An analysis of the Hirshfeld surface [5] has been executed, to understand crystal stacking, and identify the intermolecular interactions that ensure the cohesion of our crystal (fig. 2).

Key words: X-ray diffraction, crystal, Hirshfeld surface

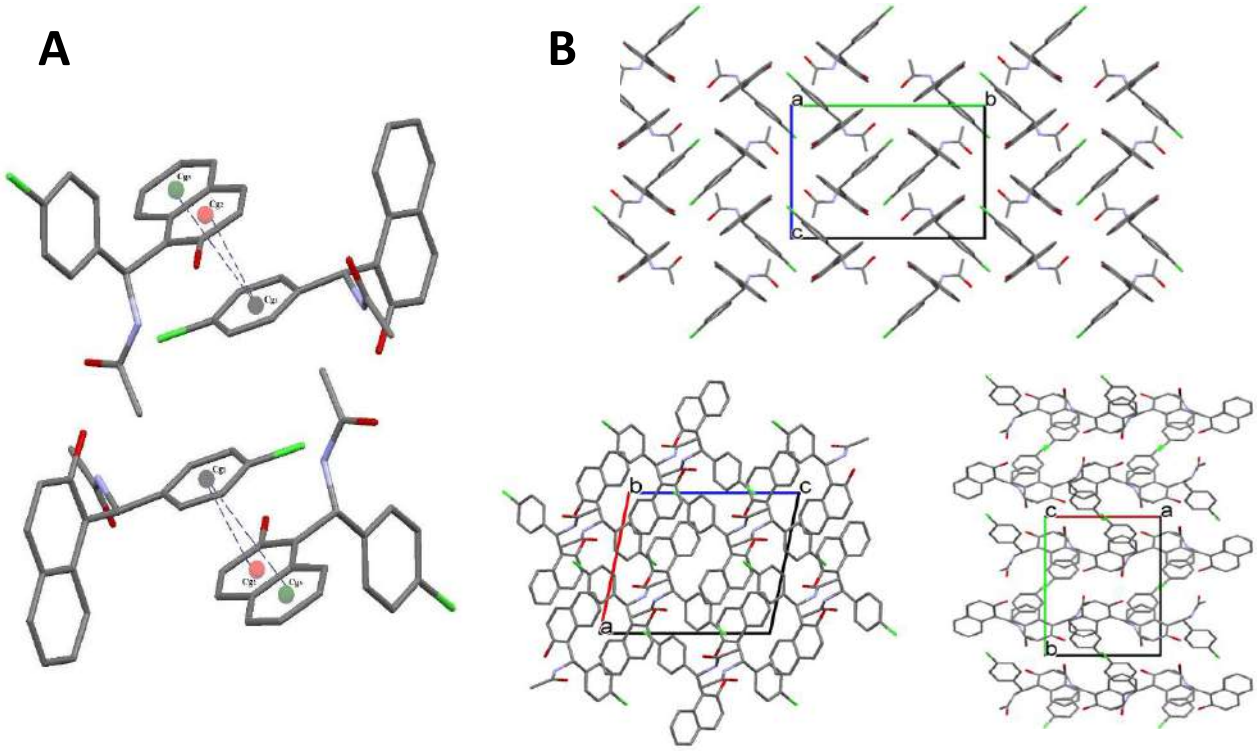


Figure 1: A : π-π interactions in CHMA *B : packing of CHMA along the three crystalorphic axis **a, b, c***

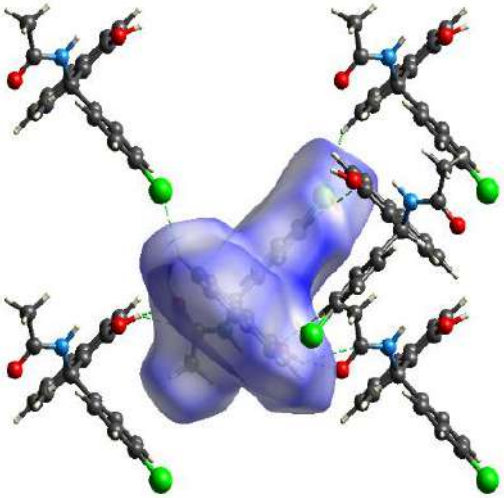


Figure 2: Hirshfeld Surface analysis with the neitghbouring molecules.

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Neutronic analysis of the Advanced Small Modular Reactor CAREM-25 by using OpenMC code

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The idea of an integrated Small Modular Reactor (SMR) is not new, but it seems that is time to put it back into the circuit within today's energy context. SMRs are defined as reactors producing an electric output power ranging between 10 MWe and 300 MWe. The International Atomic Energy Agency (IAEA) publications state that the use of these kinds of reactors has attracted the attention of many industrial countries [1].

According to the actual situation, SMRs are at different stages of design, licensing, and construction. Many technologies are proposed, including inherent concept of the widely used pressurized water reactors. The aim of this study, is to perform neutronic analysis by using OpenMC code to model and simulate the CAREM-25 reactor core (Fig.1). This open-source is based on Monte-Carlo method to simulate neutron transport and it was developed initially by researchers (CRPG) at MIT since 2011, as part of a project to develop scalable parallel algorithms for future exascale supercomputers. Indeed, by using this free and open-source code, it is possible to calculate criticality of the core, obtain the neutron flux characteristics (neutron spectrum and surface distribution) and reaction rates [2, 3].

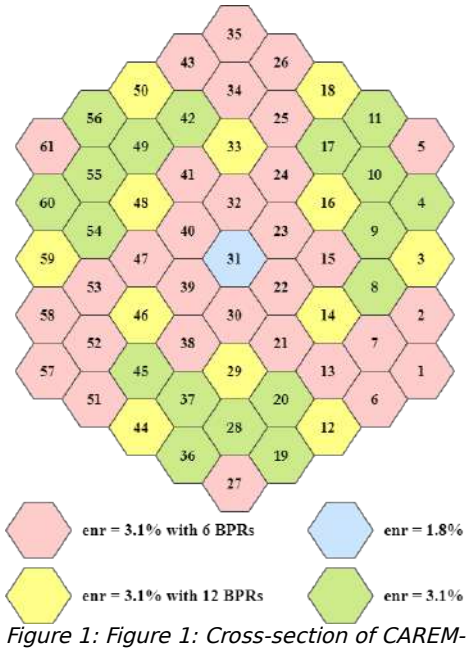


Figure 1: Figure 1: Cross-section of CAREM-25 core.

The Argentinian CAREM-25 reactor is studied here within the framework of a neutronic analysis of a configuration with standard fuel made from metallic Uranium dioxide UO_2. Initially the study was focused on a generic hexagonal fuel assembly (FA) with 108 fuel rods, then generalized to the whole core which consists of 61 fuel assemblies divided into four types according to uranium enrichment and the presence of burnable poison (Gadolinium) within some fuel rods [4].

In table 1, the most relevant geometrical characteristics and chemical composition of the reactor core components are given

Table 1. Characteristics and parameters of the CAREM-25 reactor core.

Element	***Parameter***
Active length (m)	1.4
Total length (m)	1.6
Nember of assembly	61
Nember of fuel rods per assembly	108
Nember of guide tubes	18
Nember of instrumentation tubes	1
Cladding material: Zry-4	O(0.1196%), Cr(0.0997%), Fe(0.1994%), Zr(97,1858%), Sn(1.3955%), Hf(1%)
Fuel type/assembly array	UO2 pellets/hexagonal
Coolant/ moderator	Light water
Control rod cladding material AISI 316 L	C(0.03%), Si(1%), P(0.45%), S(0.3%), Cr(17%), Mn(2%), Fe(65.395%), Ni(12%), Mo(2.5%)

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Effect of the Carreau–Yasuda rheological parameters on MHD natural convection in a square porous medium filled with (SWCNT–water) nanofluid

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The magnetohydrodynamic (MHD) natural convection of a Water (SWCNT-Water) non-Newtonian nanofluid within a square cavity filled with a saturated porous medium and exposed to a magnetic field is investigated numerically. The Dupuit–Darcy model is employed to simulate the fluid flow within the cavity, while the Carreau–Yasuda model is utilized to characterize the apparent viscosity of the nanofluid. The horizontal walls of the enclosure are maintained in an adiabatic state, whereas the other walls are subjected to differential heating. The effects of the Hartmann number (Ha) and the Carreau–Yasuda rheological parameters on fluid flow and heat transfer rates are examined. The resulting partial differential equations (PDEs) governing this problem are solved using the finite difference method (FDM), along with the appropriate boundary conditions. and the results are presented in the form of streamlines, isotherms, and contours of apparent viscosity The results indicate that an increase in the Hartmann number leads to a reduction in fluid flow and convection strength. Conversely, an increase in the fluid shear-thinning (decrease in n) results in an improvement in the rate of convection. Moreover, observed that as the value of the Hartmann number increases, the impact of the effect of the shear thinning behaviour diminishes.

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Spectroscopic properties of nuclei from ^{132}Sn mass region with Z>50 and N<82

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Researching the structure of exotic nuclei is essential for advancing our understanding of the spectroscopic properties of atomic nuclei. In this context, we have developed a new effective interaction within the shell model framework, utilizing the low-momentum potential approach to investigate nuclei surrounding 132Sn. This presentation aims to provide a versatile discussion of the energy levels, electric transitions, and magnetic moment in the isotopic chain with Z=50 and the isotonic chain with N=82, comparing our theoretical findings with available experimental data.

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Semi-empirical determination of $(L\gamma/L\alpha)$ intensity ratios in lanthanides elements

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The precise determination of X-ray intensity ratios is of considerable importance in nuclear physics, as these ratios provide valuable insights into atomic transitions and radiative processes.

This research focuses on computing semi-empirical values for the intensity ratios $(L\gamma/L\alpha)$ for elements in the atomic number range $57 \leq Z \leq 71$. The approach utilizes an interpolation technique based on the analytical function $[(L\gamma/L\alpha)_W/1\text{-}(L\gamma/L\alpha)_W]^{1/4}$, which varies as a function of atomic number Z. The experimental data is then accurately fitted to weighted average ratios, denoted as $R= (L\gamma/L\alpha)_{EXP}/(L\gamma/L\alpha)_W$. Both the experimental and weighted values are drawn from the comprehensive database compiled by Zidi et al [1]. Additionally, a detailed comparison has been made with established experimental results [2] and empirical data [3,4], showing a reasonable correlation between our findings and previous studies.

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Beyond the Burst: Light Curve Dynamics in Afterglow Emissions

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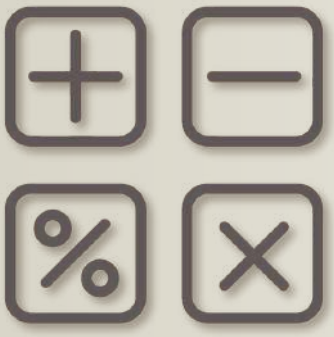
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Beyond our galaxy, **Gamma-Ray Bursts (GRBs)** are some of the brightest and most powerful events in the universe. When the source of these bursts expands and interacts with the surrounding medium, which called afterglow, that begins in X-ray frequencies and gradually shifts to radio frequencies. In this study, we simulate the light curve across this wide spectral band, using synchrotron emission as the foundational mechanism for our analysis[1,2,3].

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Afterglows (GRBs), Fire ball, Chock extern, Light curve, Synchrotron, Synchrotron Self-absorption.



MATHEMATICS

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Aperçu de la cryptographie et du codage de Lucas

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Abstract
Dans cette étude, nous nous concentrons sur l'utilisation des suites récurrentes linéaires dans le domaine du codage. Il s'agit d'abord de présenter le théorème de Zeckendorf avec la version Lucas , puis on montre comment coder et décoder un entier en utilisant la suite de Lucas classique . Enfin, on développe la partie codage en utilisant la matrice QL de Lucas (simple et généralisée) et on prouve les hautes capacités de détection et de correction basées sur le déterminant de la matrice code.

Keywords : Nombre de Lucas, Nombre de Fibonacci, Algorithme, Complexité.

Mathematics Subject Classification : 05A10, 05A17, 11B39, 14G50

1 Introduction

Depuis la découverte des suites de Fibonacci et de Lucas, les chercheurs ne cessent de découvrir de nouvelles applications de ces suites. On distinguera deux codes basés sur les nombres de Fibonacci. le premier défini par Apostolico et Frankel en 1987 dans [1], nommé le code universel de Fibonacci qui repose essentiellement sur le théorème de Zeckendorf, ce dernier propose une représentation des entiers en utilisant les nombres de Fibonacci, suivit par un préfixe. Le deuxième propose par Stankhov en 1999 dans [2], qui utilise la Qp-matrice de Fibonacci.Rachid chergui en 2020 a developer arithmétique de Zeckendorf pour les nombres de Lucas dans [6] Dans ce travail, on va développer la partie du codage en utilisant le théorème de Zeckendorf où on montrera comment coder et décoder un entier en utilisant la suite de Lucas classique, la suite Lucas d'ordre supérieur . Enfin, on va développer la partie codage en utilisant la matrice QL de Lucas.

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Exponential stabilization of the linear porous elastic materials with microtemperatures effects

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Abstract
In this paper, we study a porous-elastic system with dissipation only due to microtemperatures effect. We introduce a new stability number and prove that the unique dissipation due to the microtemperatures is strong enough to drive the system to the equilibrium state in an exponential manner. This result is new and improves previous results in the literature.

Keywords : Energy method, exponential decay, Lyapunov functional, porous system

1 Introduction

In recent years a great effort has been developed to obtain exponential stability of solutions in classical thermoelasticity and numerous stability results have been established.
In this paper, we study porous-elastic system with dissipation only due to microtemperatures effect. we use the multiplier method to prove exponential decay.
We start by introducing the energy functional of the first order.

2 Main results

In this section, we state and prove our stability result for the energy of the solution of system given by

$$\begin{cases} \rho u_{tt} = \chi u_{xx} + b\xi_x - \gamma\theta_x \\ J\xi_{tt} = k\xi_{xx} - bu_x - \beta\xi - dw_x + m\theta \\ c\theta_t = -\gamma u_{tx} - m\xi_t - k_1 w_x \\ \tau w_t = k_2 w_{xx} - k_3 w - k_1\theta_x - d\xi_{tx}. \end{cases} \tag{2.1}$$

Where $\rho, \chi, J, k, d, m, c, b, k_1, k_2, k_3, \gamma, \beta$ and τ are positive constants.
We assume that the solutions satisfy the boundary conditions and the initial data,

$$\begin{cases} u(x,0) = u_0(x), u_t(x,0) = u_1(x), \xi(x,0) = \xi_0(x), \\ \xi_t(x,0) = \xi_1(x), w(x,0) = w_0(x), \theta(x,0) = \theta_0(x), \\ u_x(0,t) = u_x(1,t) = \xi(0,t) = \xi(1,t) = 0, \forall t \geq 0 \\ \theta(0,t) = \theta(1,t) = (1,t) = w_x(0,t) = w_x(1,t) = 0, \forall t \geq 0. \end{cases} \tag{2.2}$$

Let us consider $A : D(A) \subseteq H \to H$ then the problem $(2.1) - (2.2)$ is equivalent to the abstract Cauchy problem as follows

$$U_t + AU = 0; U(0) = U_0 \in D(A) \tag{2.3}$$

Theorem 2.1. *The operator A is the infinitesimal generator of a C_0 semigroup $S(t)$ of contractions over the space H.*

So, we have the existence and uniqueness of the solution.

Theorem 2.2. *Let (u, ξ, θ, w) be a solution of the problem determined by system $(2.1)-(2.2)$. If the coefficients of the system satisfy*

$$\chi_1 = \chi - \frac{\gamma^2}{c\rho} = 0 \tag{2.4}$$

Then, (u, ξ, θ, w) decays exponentially, i.e.there exist two positive constants β_1, β_2 independent of the initial data such that

$$E(t) \leqslant \beta_1 E(0) e^{-\beta_2 t}, t \geq 0$$

So, we proved that the system $(2.1) - (2.2)$ is exeponentially stable if the condition (2.4) is verified.

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The First International Congress on Recent Advances
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Min-Max Optimal Design of a Non-Conventional Dynamic Absorber System with Negative Stiffness for Vibration Control of Damped Structures

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In this present paper, a mini-max optimal design of a non-conventional Dynamic Vibration Absorber with negative stiffness (NCNS-DVA) for damped primary structures is investigated to reduce high amplitudes in the resonant range of vibrations. The differential equation is formulated and the analytical solution of the system is derived. Using the principles of fixed-point theory, the closed-form solution for the optimal tuning coefficient is analytically obtained. Then, the optimal damping ratio and the optimal negative stiffness parameter of the proposed non-traditional DVA with negative stiffness are determined numerically by solving a set of nonlinear equations established using Chebyshev's equioscillation theorem. Extended simulations are conducted to examine the effectiveness of the optimally designed NCNS-DVA and the sensitivity of the optimal parameters. Finally, the vibration control performance of the proposed configuration is compared with those of two typical DVAs, which were presented by Liu and Pennestri, respectively. The comparison results demonstrate that the non-traditional DVA with negative stiffness significantly enhances vibration control by reducing the dynamic magnification response of damped primary structures and confining the normalized DVA stroke.

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Operational Matrix and Collocation Techniques for Fractional Volterra Equations Using Generalized Lucas Polynomials

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Abstract

In this study, we introduce a collocation approach for solving fractional Volterra integro-differential equations, utilizing generalized Lucas polynomials. The fractional derivative is formulated using the Caputo definition. By applying the operational matrix related to the fractional derivative of these polynomials, in combination with the collocation method, we reduce the problem to a system of algebraic equations. To demonstrate the validity and accuracy of the proposed method, several numerical examples are provided.

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Comparison of predictive probabilities in fully Bayesian and hybrid frequentist Bayesian approach.

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Abstract :

This paper addresses a two-step Bayesian probabilities prediction for sequential and experimental planning design. We propose the practitioner a satisfaction made by both the first and the second phase of the experiment in the case of a classical or Bayesian test study, and is predicted using the first phase. The satisfaction considered improved for its interest in the idea of satisfaction prediction and is defined as a function decreasing the probate p-values after data processing.

Our simulations are based on the binomial negative low, which assumes an infinite population size and proposes the number of failures while predicting the number of successes. At the end of our work, we have applied the results to real data in the field of finance.

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Existence of positive solution for some nonlocal elliptic problem

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Abstract

we prove existence of a positive solution to a one-dimensional nonlocal elliptic problem under weak conditions on the reaction terms and the diffusion coefficients. We use Krasnoselskii's fixed point theorem.

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A polynomial-time interior-point algorithm for solving canonical convex quadratic semidefinite optimization

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Abstract

For solving canonical convex quadratic semidefinite optimization (CCQSDO) problems, a short-step feasible full-Newton step path-following interior-point algorithm (IPA) is proposed. At each iteration, the algorithm performs only full-Newton steps with the advantage that no line search is required. Under a new selection of defaults of the threshold β which defines the wider of neighborhood of the central-path and of θ which determines the rate of decrease of the barrier parameter, we prove that the short-step IPA is well-defined and converges locally quadratically to an optimal solution of CCQSDO. Moreover, we derive its iteration bound, namely, $\mathcal{O}\left(\sqrt{m}\log\frac{m}{\epsilon}\right)$ which coincides with the best known iteration bound for such algorithms. Some numerical results are provided to evaluate the efficiency of our algorithm.

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Core Annular Flow investigated by in-House CFD Solver

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Due to the shortages of light conventional oil, the demand of heavy oil has considerably increased over the past 20 years.

And due to the high viscosity, transportation of heavy oil through pipelines became an issue to overcome and started to be a focus of many researchers these last years. One of the proposed and used solution was the Core Annular Flow – CAF - concept that uses water as an annular around the heavy oil core to reduce friction forces with the inner pipeline, pressure drop and to improve the overall system efficiency.

The performance of a numerical study of a two phase flow using a developed in-house Fortran code is evaluated in this work. The Volume of Fluid (VoF) method is used for interface tracking and the governing equations are discretised and solved using finite volume theory on a structured grid.

The code is elaborated base on SIMPLER and TDMA algorithms and used to numerically investigate the core annular flow CAF concept used for high viscosity oil pipeline transportation.

The study is conducted to track the interfaces behaviour between the two incompressible and immiscible fluids –heavy oil and water- which constitute the CAF in 2D steady and unsteady flow through a horizontal pipe while varying heavy-oil properties.

Depending on operational parameters and oil properties variation, different flow types are observed and presented in this work.

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Sliding Mode Stabilization for a class of fractional-order chaotic systems

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Keywords: Fractional-order financial chaotic system, fractional-order control, Sliding mode control, Stability.

***Abstract*—**

In this paper a fractional sliding mode controller (FOSMC) is proposed to control the chaotic fractional-order financial's system. Sliding mode control is a robust controller and it's objective is to allow the system states to move to the sliding surface and remain on it. The stability analysis for the proposed control is studied based on the Lyapunov stability theorem.

The fractional-order financial system is defined as follows [1] ,

$$\begin{aligned} X^{(q1)} &= (y-a)x + z \\ Y^{(q2)} &= 1 - by - x^2 \\ Z^{(q3)} &= -cz - x \end{aligned} \qquad (1)$$

With the parameter values given as,

$$a = 1\,;\ b = 0.1\,;\ c = 1\,;$$
$$q_1 = 1\,;\ q_2 = 0.9\,;\ q_3 = 0.8$$

To propose a sliding mode control scheme, we define the sliding surface as [2-3]

$$s(t) = D^{q_2-1}y(t) + D^{-1}\psi(t) = D^{q_2-1}y(t) + \int_0^t \psi(\tau)d\tau \qquad (2)$$

And the switching control action can be defined as follows,

$$u(t) = u_{eq}(t) + u_r(t) = -g(x,y,z) - x.f(x,y,z) - z.h(x,y,z) - Ksgn(s) \qquad (3)$$

Simulation results show the ability of the proposed controller to improve the system performance (see Figure 1).



Figure 1: Fractional-order chaotic financial system :
(a) Without control. (b) with states sliding mode control.

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Viscoelastic problem with Tresca's friction law

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Abstract

A dynamic contact problem is considered in the paper. The material is assumed to be viscoelastic with long memory in a three-dimensional thin domain Ω^{ε}. The friction is modeled with Tresca's law. The purpose of this paper is to study the asymptotic behavior of a dynamic model for frictional problem involving viscoelastic material with long memory. First, we show the variational formulation of the problem and give the existence and the uniqueness of the weak solution. Then, we use the asymptotic analysis, in which the thickness ε is the height of the domain. We establish some estimates, independent on this parameter for displacement and the velocity. The weak convergence of the velocity is proved. Finally, a generalized weak equation and the uniqueness results for the limiting problem are also proved.

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The First International Congress on Recent Advances in Mathematical, Physical and Chemical Sciences (1st-ICRAMPCS 2024) December 15-17, 2024. Constantine. Algeria

General study of a modified chaotic model

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In this work we present a theorical study of a new chaotic model wich is a modified rossler model. Analytic and numerical results shown in this paper.

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Finite Difference method for Solving Heat Equation: Codes Matlab

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Abstract

In this paper, we present a mathematical model for solving heat equation submitted to boundary conditions and initial condition. First, we construct a numerical scheme and we associated all conditions in our NS. Second, we study the stability, consistence and convergence of our NS. Some numerical results are presented at the end of this work.

1 Introduction

Let N and M be two positive integers and assume that the space step and time step are $h = \frac{1}{N}$ and $k = \frac{T}{M}$ respectively. Define $\Omega_h = \{(x_i, t_j) \mid x_i = ih,\ t_j = jk,\ 0 \leq i \leq N,\ 0 \leq j \leq M\}$. In this paper, we consider the finite difference discretization for the following initial boundary value problem of wave equation in aera $\Omega = (0, 1)$ and $t \in (0, T)$. Mathematically, the wave equation is a hyperbolic partial differential equation of second order. The wave equation looks like this:

$$\frac{\partial u}{\partial t}(x, t) = \alpha \frac{\partial^2 u}{\partial x^2}(x, t), \tag{1.1}$$

the Dirichet boundary conditions are given by

$$u(0, t) = u(1, t) = 0, \forall t \in (0, T), \tag{1.2}$$

and the initial condition is

$$u(x, 0) = 0, \forall x \in (0, 1), \tag{1.3}$$

where α is nonzero constant coefficient.

Matlab code for example

```
%The program solves the heat eq. p*du/dt- k*u''=f(x,t), %u(0,t)=20, and u(10,t)=70,
%u(x,0)=sin(pi*xx/2)+5*xx+20, %f(x,t)=0, %k=1 and p=1. clear all clc format long k=1; p=1; x_Int=[0 10];
%Space interval t_Int=[0 1]; % time interval n=20; % n is the number of subintervals for the spatial
variable a=x_Int(1); b=x_Int(2); h=(b-a)/n; xx=a:h:b; % The partition of the time interval
nn=5; % nn is the number of subintervals for the time aa=t_Int(1); bb=t_Int(2); hh=(bb-aa)/nn;
tt=aa:hh:bb;
%Computing the mass matrix M000 M000=zeros(n-1,n-1); for i=1:n-1 M000(i,i)=4; end for i=1:n-2
M000(i,i+1)=1; M000(i+1,i)=1; end M000=(h/6)*M000;
 %computing the stiffness matrix M110 M110=zeros(n-1,n-1); for i=1:n-1 M110(i,i)=2; end for i=1:n-2
M110(i,i+1)=-1; M110(i+1,i)=-1; end M110=(1/h)*M110; %Computing the loud vector bb00
bb00=zeros(n-1,1); bb00(1,1)=k*20/h; bb00(n-1,1)=k*70/h;
```

Conclusion

In this work we presented some basic and general theory of the finite difference method. We also discussed the numerical scheme and discretization of one and two dimensional problems. After that, the error estimation in its both types, a posteriori and a priori is explained. At the end, we talked about numerical examples in one and two dimensions using MATLAB software, where figures for the exact and approximate solutions with the corresponding errors are provided and explained.

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The First International Congress on Recent Advances in Mathematical,
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Divergences based Bayesian estimation with censored data

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Abstract

Bayesian techniques constitute a very important part of statistical inference since they allow to use the preliminary information about the distribution of interest through the prior distributions. On the other hand, divergences between measures represent a useful tool in statistics. They permit to construct robust estimators and tests. Many works in the literature deal with the application of divergences in statistics. For example, [3] proposed dual $\phi-$divergence Bayes type estimators for parametric models in the case of complete data. He also established their asymptotic normality. For our part, we extend the results of [3] to the case of right censored data.
To be able to define our proposed estimators, we need to introduce some notations. Let X be a non-negative real random variable (r.r.v.) of interest. We assume that X is right censored by a non-negative r.r.v. R, independent of X. So, instead of observing X, we observe a sample $(Z_i = \min(X_i, R_i), \Delta_i = 1_{\{X_i \leq R_i\}})_{1 \leq i \leq n}$ ($1_{\{.\}}$ denotes the indicator function) of independent and identically distributed copies of the pair $(Z = \min(X, R), \Delta = 1_{\{X \leq R\}})$. For any right continuous function $K : \mathbb{R} \longrightarrow \mathbb{R}$, we set $K(x^-) = \lim_{\varepsilon \geq 0} K(x - \varepsilon)$ and $\Delta_K(x) = K(x) - K(x^-)$ whenever the limit exists. Since X is not completely observed, we estimate F_X by the well known Kaplan-Meier estimator, defined by

$$F_n(x) = 1 - \prod_{i/Z'_i \leq x} \left(1 - \frac{D(Z'_i)}{U(Z'_i)}\right),$$

where $(Z'_i)_{1 \leq i \leq m}$ $(m \leq n)$ are the distinct values in increasing order of $(Z_i)_{1 \leq i \leq n}$, $D(Z'_i) = \sum_{j=1}^{n} \Delta_j 1_{\{Z_j = Z'_i\}}$ and $U(Z'_i) = \sum_{j=1}^{n} 1_{\{Z_j \geq Z'_i\}}$.
The empirical measure of F_n, denote it $\mathbb{P}_n^{KM}$, can be written as

$$\mathbb{P}_n^{KM} = \sum_{i=1}^{m} \Delta_{F_n}(Z'_i)\, \delta_{Z'_i} = \sum_{i=1}^{n} \frac{\Delta_{F_n}(Z_i)}{D(Z_i)}\, \delta_{Z_i},$$

δ_x being the Dirac measure which puts all the mass at the point x, for all x.
We assume that the distribution of X belongs to a parametric family $\{P_\theta, \theta \in \Theta\}$, where Θ is a

compact set of $\mathbb{R}^d$. We also assume that this parametric family is dominated by a $\sigma-$finite measure μ and we denote by $p_\theta = \dfrac{dP_\theta}{d\mu}$ the Radon-Nikodym derivative of P_θ with respect to μ. Let θ_T be the true value of θ and let $\phi : \mathbb{R} \longrightarrow [0, +\infty]$ be a strictly convex function of class $\mathcal{C}^2$ such that $\phi(1) = 0$. Furthermore, let π ba a prior density on Θ, following [3], we define the dual $\phi-$divergence Bayes type estimators of θ_T by

$$\widehat{\alpha}^*_\phi(\theta) = \frac{\int_{\mathcal{U}_\theta} \alpha \exp\{n\mathbb{P}_n^{KM} h(\theta, \alpha)\}\pi(\alpha)\, d\alpha}{\int_{\mathcal{U}_\theta} \exp\{n\mathbb{P}_n^{KM} h(\theta, \alpha)\}\pi(\alpha)\, d\alpha},$$

where

$$h(\theta, \alpha) : \mathbb{R}_+ \longrightarrow \mathbb{R}$$
$$x \mapsto h(\theta, \alpha, x) = \int \phi'\left(\frac{p_\theta}{p_\alpha}\right) p_\theta - \left[\frac{p_\theta(x)}{p_\alpha(x)}\phi'\left(\frac{p_\theta(x)}{p_\alpha(x)}\right) - \phi\left(\frac{p_\theta(x)}{p_\alpha(x)}\right)\right],$$

$\mathbb{P}_n^{KM} h(\theta, \alpha) = \int h(\theta, \alpha)\, d\mathbb{P}_n^{KM}$ and $\mathcal{U}_\theta = \{\alpha \in \Theta \text{ such that } D_\phi(P_\theta, P_\alpha) < \infty\}$ ($D_\phi(P_\theta, P_\alpha) = \int \phi\left(\dfrac{p_\theta(x)}{p_\alpha(x)}\right) p_\alpha(x)\, dx$ being the $\phi-$divergence between P_θ and P_α).
In the present work, we establish the asymptotic normality of $\widehat{\alpha}^*_\phi(\theta)$. We also illustrate the performances of these estimators through a simulation study and some applications on real data.
Keywords:
Bayesian estimation, Divergences, Duality, Censored data, Asymptotic normality

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The First International Congress on Recent Advances in Mathematical,
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Reliability of $(n, f, k) : F$ system with sparse d for Markov-dependent components

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Abstract

A linear $(n, f, k) : F$ system with sparse d was introduced by Zhao et al. [1], where they studied its reliability in the case of independent and identical components by employing the finite Markov chain imbedding technique. In this paper, we consider the situation where the components of the system are non-homogeneous Markov dependent, and we derive a closed-form formula for the reliability of the system using the probability generating function method. Finally, we present a numerical example to facilitate the use of the formula.

Keywords: reliability, Markov-dependent, probability generating function

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REGULARIZATION METHOD FOR A CLASS OF INVERSE PROBLEMS OF PARABOLIC DIFFERENTIAL OPERATOR EQUATION

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Abstract

The present paper introduces a modified regularization method for an ill-posed Cauchy problem that has an unbounded linear and self-adjoint positive operator with a discrete spectrum. The method used here consists of perturbing both the equation and final condition to obtain an approximate nonlocal problem depending on two small parameters. We demonstrate its stability and is approaching the solution of the original problem.

We shall consider the final value problem $u : [0, T] \to H$ such that

$$\begin{cases} u'(t) + Bu(t) = 0 \quad 0 \leq t < T \\ u(T) = \psi. \end{cases} \tag{0.1}$$

with the final value ψ in H. This problem is ill-posed, often the unique solution exists on $[0.T]$, but it does not depend continuously on the given final value. There have been many methods to regulate it. We cite the quasi boundary value method (QBVM) see [3] and the quasi reversibility method (QRM) see [1]. The regularization method used in this work hybridizes elements of the (QRM) and the (QBVM). It was developed in [2], in the continuous case. In this work, we state the discrete case.

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Bounds for Consecutive k-out-of-n: G Systems with Dependent Components

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Abstract:

The main purpose of our paper is to establish upper and lower bounds for a consecutive k-out-of-n: G system where the components are dependent with arbitrary distributions functions.

First, we present the new bounds for the system under consideration. Then, we compare our bounds with several existing bounds over numerical results and graphical representations.

At the end, discussions are made to show the advantages of the proposed bounds.

Keywords: reliability, consecutive, dependent, upper bound, lower bound.

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Asymptotic normality of the kernel estimator of the conditional distribution for functional and right-censored data

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Abstract

Nonparametric estimation is a vital aspect of modern statistics, offering powerful techniques for analyzing data without relying on specific parametric assumptions about the underlying distributions. This flexibility is particularly advantageous for estimating conditional distributions, allowing for a nuanced analysis of how one variable can predict another, typically aiming to forecast the response variable Y based on the explanatory variable X. Recent literature has increasingly focused on models tailored for infinite-dimensional (functional) data. Notably, [1] demonstrated the almost complete convergence of the conditional distribution estimator, while [2] established the asymptotic normality of the estimator for the conditional distribution function under the assumption of quasi-associated observations.
However, complete data for Y is often unavailable in many scientific fields, prompting researchers to work with incomplete data, which can be categorized into two types: truncated data and censored data. Right censoring is the most frequently encountered issue in survival data collection and has garnered considerable attention in the literature. We refer to [3], which discusses the asymptotic normality of local linear estimation for the conditional cumulative distribution function.
In our study, we focus on estimating the conditional distribution when the response variable is right-censored and the explanatory variable is functional. We also established the asymptotic normality with explicit rates for the constructed estimator.

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Hom-action and Hom-Bi-action With Applications 1^{st}-ICRAMPCS 2024

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Abstract

The Hom-groups' category differs from the groups' category. The Hom-group is a nonassociative structure that generalizes the notion of groups. We obtain the operation by composing it with a multiplicative mapping that changes the associativity axiom with another condition called the twisting form. The present exposes the different notions of Hom-actions and Bi-actions concerning Hom-groups. In addition, we show the validity of certain important theorem known in the classic case, in particular, the First Sylow Theorem, and normalizer lemma, and illustrate the results by giving some applications for the finite case.

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RFE-SVM: An Approach to Enhancing Support Vector Machine Performance through Recursive Feature Elimination.

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Abstract

This study explores the effectiveness of Recursive Feature Elimination (RFE) in enhancing the performance of Support Vector Machine (SVM) classifier for binary classification tasks. Feature selection is crucial for improving model performance, as it reduces complexity and emphasizes significant variables. We implemented data preprocessing techniques to prepare the data before applying RFE to identify the most relevant features for the SVM and compared its performance with that of logistic regression and Naive Bayes classifiers. The results indicated that the RFE-SVM outperformed both of them across multiple evaluation metrics, including accuracy, precision, recall, and F1 score. This research demonstrates that RFE is a powerful method for improving the performance of SVM classifier, underscoring the importance of robust feature selection in machine learning.

Keywords : Classification,Feature selection, Recursive Feature Elimination, Support Vector Machine.

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The Relation Between the Numerical Range of Tow Sub-Self-Adjoint Operators

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Abstract

In this paper we determine necessary and sufficient conditions such that the numerical range of a bounded linear operator $A \in B(H)$ is a line segment.
We present a new set **S**, such that **S** is a set of operators where the numerical range $W(A)$ is a line segment, the support for this line segment is given by the following equation: $Y = aX + b$ such that **a**: The slope of the straight line, **b**: is a constant.
The set **S** is of the following form

$$S = \{A \in B(H) , \exists (\lambda, \mu) \in \mathbb{C}^2; A* = \lambda A + \mu I\}$$

Now, we show that the set **S** is invariant by unitary equivalence, and we given some properties related of the set **S**.
On the other hand, we investigated the relation between the numerical range of tow sub-self-adjoint operators.

Keywords: Numerical Range, Numerical Radius, Self-Adjoint Operator.

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Hopf bifurcation in a predator-prey biological economic system with a nonlinear harvesting rate.

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Abstract

This research examines the stability and Hopf bifurcation of a biological economic system involving harvesting efforts on prey. The model under consideration is characterised by differential-algebraic equations due to economic income. We select economic income as a favourable bifurcation criterion in this context. This model, characterised by a nonlinear harvesting rate, is more comprehensive than the models proposed by earlier researchers. Moreover, the enhanced parameterisation calculation procedure is far more straightforward and capable of managing more intricate models that were previously unmanageable due to substantial computational demands. The validity and viability of the results gained are demonstrated through MATLAB simulation.

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Recovering Steklov Parameters and Boundary Conditions in the Forth Order Partial Differential Equation Using Incomplete Cauchy Data.

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Abstract

This paper investigates an inverse problem related to the forth order partial differential equation within a simply connected, bounded domain, with the objective of completing the missing Cauchy data and determining unknown parameters on a non-measurable boundary portion subjected to Steklov boundary conditions. The approach involves reformulating the problem into a set of non-linear, ill-posed boundary integral equations that faithfully represent the original inverse problem. To address the challenge posed by incomplete Cauchy data, we employ Tikhonov regularization coupled with a minimization technique to achieve a robust solution. The proposed methodology is validated through a series of numerical experiments, showcasing its reliability and accuracy in data completion problem and parameters recovery.

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The Bayes factor for evaluating disparities in cure percentages within survival curves

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Abstract

A specific kind of survival analysis model known as a "cure model" makes the assumption that a given percentage of individuals will never encounter the event and that, as a result, the survival curve will plateau. According to population-based cancer studies, a cure is achieved when the group of ill people's mortality rate (or risk) approaches the level predicted for the general population. In cancer, comparing cure rates enables us to evaluate therapy efficacy and choose the best therapeutic approaches to increase patient longevity. By accounting for unique cancer traits and risk factors, it also aids in personalising care. In this work, we investigate colorectal cancer in Constantine, Algeria. We estimate the cure rates for each form of colorectal cancer using a well-known distribution—the exponential distribution. In order to provide quantitative statistical evaluations of the difference in cure rates, we then run statistical tests using the Bayes factor and the Savage-Dickey ratio, which is thought of as a direct technique of comparison.

Keywords: Cure models, Bayes factor, colorectal cancer.

1 Introduction

In the field of survival statistics, the cure fraction plays a crucial role, particularly in oncology studies where it is common to find that some patients do not experience disease recurrence after treatment. The cure fraction survival model (or “cure fraction” model) allows to take into account the possibility that a subset of patients is definitively cured, i.e. they are no longer likely to experience the event of interest (e.g., relapse or death due to cancer). Statistically, this model enriches the analysis by introducing a clear distinction between cured patients and those who remain at risk, which improves the accuracy of long-term survival predictions.

In oncology, the cure fraction is of particular importance for assessing the efficacy of treatments, including chemotherapies, radiotherapies, and immunotherapies. In these models, the cure fraction measures the proportion of patients for whom the treatment is truly curative, a key indicator of therapeutic success. This approach also allows examining the impact of risk factors or individual characteristics on the probability of cure, thus contributing to personalized care. By integrating this cure fraction into survival models, researchers and clinicians can obtain a more complete view of patient prognosis, which is essential for improving treatment strategies in oncology. Various approaches, both parametric and non-parametric, have been considered to model the proportion of immunes and interested readers are referred to, for example, Boag (1949), Berkson and Gage (1952), Haybittle (1965), Farewell (1982, 1986), Copas and Heydari (1997), Ng and McLachlan (1998), De Angelis et al. (1999), Sy and Taylor (2000), Balakrishnan and Pal (2013).

Comparing cure rates between two survival functions is of paramount importance in oncology, where treatment evaluation is often based on their ability to prolong patients' lives and induce a

durable cure. Indeed, in the context of cancers, patient follow-up after treatment can reveal complex survival dynamics, with one subgroup potentially cured, while another remains at risk of recurrence. Survival models with cure fraction, which differentiate these groups, provide an essential perspective for understanding the effects of therapeutic interventions in the long term. Comparing cure rates between two groups, whether patients on standard and experimental treatment or different clinical cohorts, helps to assess the relative efficacy of treatments and guide clinical decisions. This approach also allows to analyze survival differences according to individual patient characteristics, thus contributing to the personalization of oncology care. Bayesian statistics plays a fundamental role in the analysis and comparison of cure rates between two survival functions, particularly in the field of oncology. Unlike the classical frequentist approach, which relies on fixed assumptions and significance tests, the Bayesian approach allows to explicitly incorporate prior knowledge in the form of prior distributions, while updating this knowledge using observed data. This Bayesian framework is particularly suited to the estimation of survival models with cure fraction, where a proportion of patients can be considered definitively cured. Using Bayesian tools, it is possible to model uncertainty around key parameters, such as cure rates or recurrence risks, and to obtain posterior distributions that reflect all available information. In oncology, where data may be limited or heterogeneous, this approach allows for greater flexibility, while facilitating comparisons between different patient groups or treatments. Thus, Bayesian statistics offers a powerful methodology to improve clinical decision-making, enabling more nuanced and probabilistic analyses of cure rates.

In this work, we use a well-known distribution, which is the exponential distribution, to estimate the cure rates for each type of cancer and then perform the following two tests:

- Hypothesis test 1 (equality between healing fractions)

$$\begin{cases} \mathcal{H}_{01} & p_0 = p_1 \\ \mathcal{H}_{11} & p_0 \neq p_1 \end{cases} \qquad (1)$$

- Hypothesis test 2 (difference in fractions is Δ)

$$\begin{cases} \mathcal{H}_{02} & p_0 - p_1 = \Delta \\ \mathcal{H}_{12} & p_0 - p_1 \neq \Delta \end{cases} \qquad (2)$$

Thanks to the Bayes factor, a statistical evaluation can be given for the difference between the cure rates, such that $p0$ is the cure fraction for the colon cancer group and $p1$ is the cure fraction for the rectal cancer group. Although the problem of parameter estimation has been largely solved by the progress of Markov Chain Monte Carlo (MCMC) methods, the calculation of this factor remains complicated. Several calculation methods have been proposed to solve these problems. In this work, we propose a Bayes factor analysis based on the Savage-Dickey density ratio (Dickey, 1971, Dickey & Lientz, 1970). The interest of this method is the possibility of implementing the test with the MCMC method.

2 Main results

In our application, we found a significant difference in terms of cure although the two survival curves for the two types of colorectal cancer are not statistically different in terms of hazard functions. Through statistical tests, we found that in the long term, the difference in cure rates between colon cancer and rectal cancer reaches 10 with statistical significance, which cannot be discovered by any other known method. This result implies the importance of these tests to enrich the survival analysis and to give a statistical quantification based on the Bayes factor table for the differences between cure rates. In addition, the Dickey – Savage method offers practical, simple

and relatively easy solutions because of the direct use of the results of Monte Carlo sampling by Markov Chains. Finally, through this work, we can conclude the major role attributed to point tests, more practical in the field of survival compared to other models and hypotheses due to the small difference between the intervals.

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Complex dynamics and chaos in a fractional-order discrete-time SIS epidemic model

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Abstract

In this work, a fractional-order discrete-time SIS epidemic model is presented. The Caputo-like discrete operator is employed to construct the fractional-order epidemic model. The stability of equilibrium points of the model is analyzed. Furthermore, the existence of chaos in the proposed model is confirmed via several nonlinear powerful tools, such as phase plots, bifurcation diagrams, and the maximum Lyapunov exponent spectrum. Using these tools, we have established that the SIS model can exhibit complex dynamics and unpredictable behavior. An active nonlinear controller has been designed to stabilize the chaotic motions in the fractional-order SIS epidemic model.

Keywords: SIS model, Caputo-like operator, Chaos, Stabilization.

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Statistical analysis of spatio-temporal bilinear processes

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Abstract

In this paper, we define a spatio-temporal model with location dependent parameters to describe temporal with variation and spatial nonstationarity. We consider the prediction of observations at unknown locations using known neighbouring observations. Further we propose a local least squares based method to estimate the parameters at unobserved locations. The sampling properties of these estimators are investigated.

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An overview on modeling techniques and the accuracy measures with an application example

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Abstract Big Data poses a huge burden in terms of storage, communication, analysis and modeling. It has given birth to data science that deals with these burdens. Metamodel (Computer experiments) is the analysis, construction, and development of the frameworks, constraints, models and theories that are applicable and useful for modeling a predefined class of problems in physics, chemistry, climatology, astrophysics, and biology, human systems in social science, etc. Modeling is the process of describing a real-world problem in mathematical terms, usually in the form of equations. It involves using mathematical concepts and languages to represent concrete systems in abstract way. How to find the best suited metamodel is another key issue in computer experiments. Various modeling techniques have been proposed, such as linear regression model, polynomial regression model, spline model, and Kriging (spatial correlation) model. As well as variable selection techniques, including AIC, BIC, RIC, SCAD, and LASSO. For testing the accuracy of the metamodel, the mean square errors (MSE), R^2, R^2_{adj} and others are the widely used measures. In this work, to illustrate the modeling technique, we perform metamodel tool with a variety of real models.
Keywords: Accuracy measures, metamodel, modeling techniques

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Generating functions of the triple product of Padovan number with square well-known Gaussian numbers.

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Abstract

In this article, we introduce new generating functions for the triple product Padovan number, with some square well-known Gaussian numbers, by making use of the symmetrizing endomrphism operator $\delta^k_{b_1b_2}\delta^h_{c_1c_2}$ to the series $\sum_{n=0}^{\infty} S_n(A)b_1^n c_1^n z^n$.

Keywords: Padovan number, Gaussian numbers, Generating function, Symmetric function.

1 THEOREMS and MAIN RESULT

Theorem 1.1. *Given three alphabets* $A=\{a_1,a_2,a_3\}$, $B=\{b_1,b_2\}$ *and* $C=\{c_1,c_2\}$, *then we have*

$$\frac{\sum_{n=0}^{\infty} S_n(A)S_{n+k-1}(B)S_{n+h-1}(C)z^n}{\left(\sum_{n=0}^{\infty} S_n(-A)b_1^n c_1^n z^n\right)\left(\sum_{n=0}^{\infty} S_n(-A)b_1^n c_2^n z^n\right)\left(\sum_{n=0}^{\infty} S_n(-A)b_2^n c_1^n z^n\right)\left(\sum_{n=0}^{\infty} S_n(-A)b_2^n c_2^n z^n\right)}$$

$$= \frac{c_1^h c_2^h}{(b_1-b_2)}\left(\begin{array}{l}\sum_{n=0}^{\infty} S_n(-A)S_{n-h-1}(C)b_2^{n+k}z^n \sum_{n=0}^{\infty} S_n(-A)b_1^n c_1^n z^n \sum_{n=0}^{\infty} S_n(-A)b_1^n c_2^n z^n \\ -\sum_{n=0}^{\infty} S_n(-A)S_{n-h-1}(C)b_1^{n+k}z^n \sum_{n=0}^{\infty} S_n(-A)b_2^n c_1^n z^n \sum_{n=0}^{\infty} S_n(-A)b_2^n c_2^n z^n\end{array}\right) \quad (1.1)$$

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Comparative Analysis of Electromagnetic Fields in Flat vs. Curved Spacetime Using Maxwell's Equations

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This paper presents a comparative analysis of Maxwell's equations in flat space and curved spacetime to gain insights into the behavior of the electromagnetic field under gravitational influence. By numerically solving these equations in both contexts, we explore how the geometry of spacetime impacts electromagnetic wave propagation, with a central focus on the Gaussian impulse function, a common model for mathematical modelling in Engineering and transport phenomena, offering valuable contributions to the understanding of transport phenomena in curved geometries.

The Gaussian pulse generation [1] is created using the formula:

- $G(t) = A.\exp\left(-\frac{\left(t-t_{peak}\right)^2}{2\sigma^2}\right)$

Where A is the amplitude of the pulse (e.g.,1000), t_{peak} is the time at which the pulse reaches its peak (e.g., ($100/3.10^8$) seconds), σ is the standard deviation, representing the width of the pulse (e.g.,$2.5.10^{-9}$ seconds).

In flat space, Maxwell's equations [2] are expressed as:

- $\nabla.E = \frac{\rho}{\varepsilon_0}$
- $\nabla.B = 0$
- $\nabla \times E = -\frac{\partial B}{\partial t}$
- $\nabla \times B = \mu_0 J + \mu_0 \varepsilon_0 \frac{\partial E}{\partial t}$

Where E and B represent the electric and magnetic fields, ρ is the charge density, J is the current density, ε_0 and μ_0 are the permittivity and permeability of free space, respectively. These equations describe how electric and magnetic fields propagate and interact in the absence of material media.

In curved spacetime, Maxwell's equations are modified [3] to incorporate the effects of spacetime curvature to account for gravitational effects.

- $\nabla_\mu F^{\mu\upsilon} = \frac{1}{\sqrt{-g}}\partial_\mu\left(\sqrt{-g}F^{\mu\upsilon}\right) = \frac{J^\upsilon}{c}$
- $\nabla_\lambda F^{\mu\upsilon} = 0$

Where $F^{\mu\upsilon}$ is the electromagnetic field tensor and g is the determinant of the metric tensor $g^{\mu\upsilon}$, which describes the curvature of spacetime. The introduction of the metric tensor modifies the divergences and curl operations, reflecting how electromagnetic fields are influenced by the geometry of spacetime. The indices μ *and* υ indicate the components of the tensor in four dimensional spacetime. The term $\sqrt{-g}$ appears when converting between coordinate volumes in curved spacetime. It's a factor used to ensure that integrals over spacetime remain invariant under coordinate transformations. Following this theoretical

framework, the Gaussian pulse plot is shown in Figure 1, highlighting the pulse's distinct shape with amplitude on the y-axis and time on the x-axis. This representation is crucial for understanding transient electromagnetic phenomena.

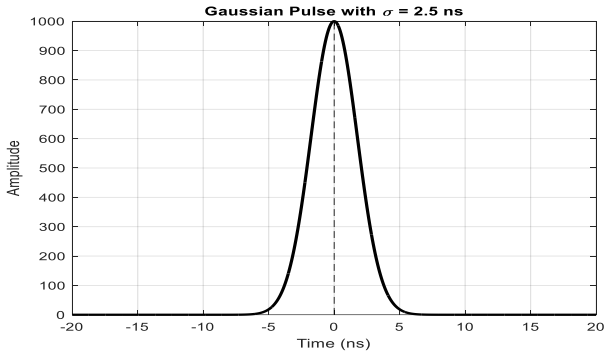


Figure 1: Gaussian pulse.

Figure 2 (a) and (b) show a comparison of Maxwell's equations, representing the electric and magnetic fields in both flat spacetime and curved spacetime.

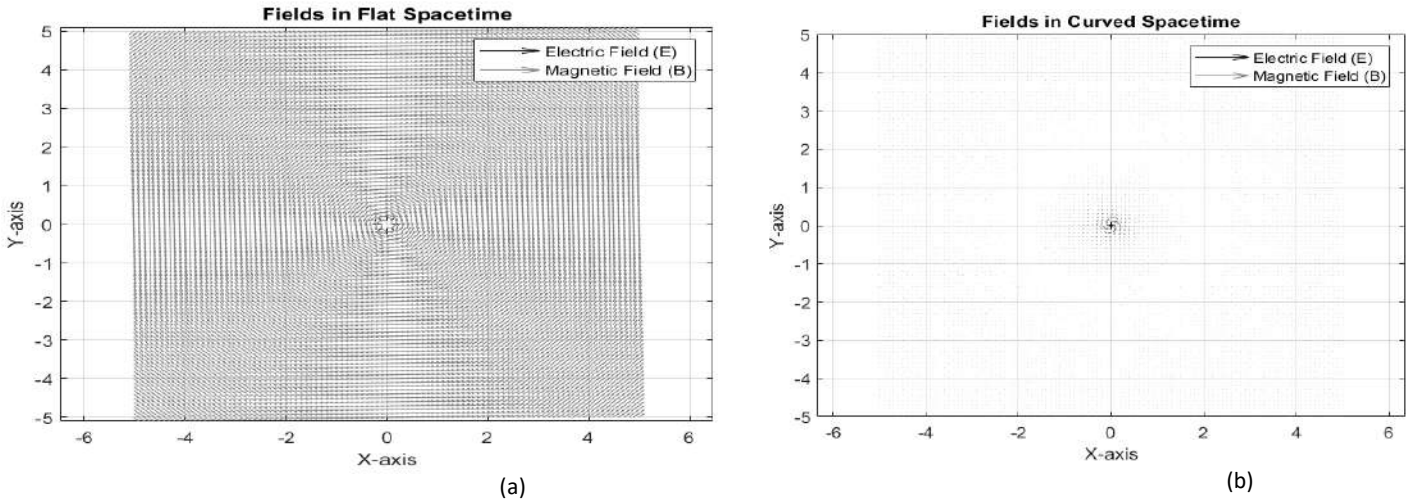


Figure 2: Comparing Maxwell's equations in (a) flat spacetime and (b) curved spacetime

In flat spacetime (Figure 2 (a)), field lines are uniform, symmetric, and unaffected by gravitational influences, allowing electromagnetic fields to propagate freely in all directions according to classical Maxwell's equations. However, in Curved spacetime (figure 2 (b)), field lines are curved and distorted by spacetime, showing the influence of spacetime on electromagnetic fields.

Overall, when modified for curved spacetime, Maxwell's equations reflect the fundamental connection between electromagnetism and gravity. This is important to understand the transport phenomena, especially how electromagnetic fields influence the movement of charged particles and energy transfer in various systems.

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Comparative Analysis of Autoencoder Variants for Image Reconstruction Using the Olivetti Face Dataset

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Abstract

This study offers a detailed comparative analysis of different autoencoder variants for image reconstruction, using the Olivetti face dataset. The analysis covers Autoencoder, Variational Autoencoder (VAE), and Convolutional Autoencoder (CAE) to assess their effectiveness in reconstructing facial images. The Olivetti face dataset, consisting of 400 grayscale images of 40 individuals, is used as the evaluation benchmark. The AE and CAE are constructed with fully connected and convolutional layers, respectively, while the VAE incorporates variational techniques to learn a latent representation of the data. The experimental process includes preprocessing the dataset, training each autoencoder variant, and evaluating their performance using metrics like Mean Squared Error (MSE) and Structural Similarity Index (SSIM). The results reveal that although all autoencoder variants exhibit strong reconstruction capabilities, the CAE excels in both quantitative metrics and visual quality of the reconstructed images. This study underscores the strengths and weaknesses of each autoencoder variant, offering valuable insights for future research and applications in image reconstruction and related domains.

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The strong consistency of the kernel conditional distribution estimator

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Abstract

Considering the Nadaraya-Watson kernel estimator we aiming to explore its asymptotic properties, with a particular emphasis on the conditional distribution estimator for independent and identically distributed (i.i.d.) data. Our main objective is to demonstrate the almost complete convergence of the kernel conditional distribution estimator, providing a comprehensive theoretical framework for analyzing its behavior. To complement these theoretical findings, we carry out an extensive simulation study that illustrates the estimator's practical utility and performance. This research sheds light on the estimator's consistency and efficiency across various scenarios, offering valuable contributions to the field of nonparametric estimation.

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Finite-Time Projective Synchronization of Fractional-Order Chaotic Systems with Different Structures

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Abstract

This paper investigates the finite-time projective synchronization of two fractional-order chaotic systems with different structures. By employing finite-time stability theory, several judgment criteria for synchronizing these systems are derived and proven. A novel controller is proposed to achieve finite-time generalized projective synchronization, offering a faster convergence rate for error systems and practical ease of implementation in engineering applications. The effectiveness and feasibility of the proposed synchronization strategy are further validated through numerical simulations, which confirm the theoretical results and demonstrate the practical utility of the approach.

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Asymptotic study of Local linear predictor for time series

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The non-parametric estimation plays a fundamental role in explaining existing knowledge and developing new theories based on observations.

Important decisions in different fields are particulary based on forecasting models, when investigating the link between two real variables X the covariate and Y the target, using kernel methods.

The popularity of such estimates can be attributed to their flexible nature, as well as their various computational issues. We focus here on a polynomial of degree one and we deal then with the local linear least squares kernel regression estimator. It is known to have optimal rates of convergence, another important advantage is that the asymptotic bias appears to be superior to those of the Nadarya-Watson or Gasser-Muller kernel estimators. Moreover, it is shown that the local linear regression estimate has a good behavior for both random and fixed regression models.

We are interested here to the consistency of the local linear predictor in the context of time series. We give the almost complete convergence of the local linear regression estimator, noting that it is stronger than the almost sure one. We specify additionally the rate of this convergence.

In [1], the local linear regression estimator is studied and compared to Nadaray-Watson estimator in the case of functional dependent data,
Other kernel estimators are studied for dependent data, we cite among others [2], where the strong consistency of a recursive regression estimator is studied for a generalized structure of dependent data.

As an application of local linear estimation of the regression function, we choose to predict future values of an autoregressive time series fulfilling the condition of strong mixing, this allows to validate the studied convergence result.

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ON CERTAIN $D(9)$ AND $D(64)$ DIOPHANTINE TRIPLES

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Abstract

A set of m integer $\{a_1, \cdots, a_m\}$ is called a Diophantine m-tuple with property $D(\ell)$, or alternatively a $D(l) - m$-tuple, if $a_i a_j + \ell$ is a perfect square for any distinct $i, j \in \{1, 2, ..., m\}$. Fermat showed that the set $\{1, 3, 8\}$ can be extended from a $D(1)$-triple to a $D(1)$-quadruple with the additional element 120. Baker and Davenport showed that 120 is in fact the only integer that extends this set from a $D(1)$-triple to a $D(1)$-quadruple. This was also the first appearance of the method that came to be known as Baker-Davenport Reduction. A result of Bać ić and Filipin characterizes the solutions of Pellian equations that correspond to $D(4)$-Diophantine triples of a certain form.

We generalize this result in order to characterize the solutions of Pellian equations that correspond to $D(\ell^2)$-Diophantine triples. Motivated by thise result and bounds on linear forms in logarithms of algebraic numbers in order to classify all $D(9)$ and $D(64)$-Diophantine triples of the form $\{F_{2n+8}, 9F_{2n+4}, F_k\}$ and $\{16F_{2n+6}, F_{2n+12}, F_k\}$, where F_i denotes the i^th Fibonacci number.

The Fibonacci numbers are defined by the recurrence relation:

$$F_{n+1} = F_n + F_{n-1} \text{ with } F_1 = F_2 = 1,$$

the sequence of Fibonacci numbers is seen to be as follows, $1, 1, 2, 3, 5, 8, 13, 21, 34, \ldots$.

The n^{th} term of this sequence is given by is called Binet's formula,

$$F_n = \frac{\alpha^n - \overline{\alpha}^n}{\sqrt{5}} \quad \text{where} \quad \alpha = \frac{1+\sqrt{5}}{2} \quad \text{and} \quad \overline{\alpha} = \frac{1-\sqrt{5}}{2}.$$

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Solving a family of transmission boundary problems governed by complet elliptic differential equations in UMD spaces

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Abstract : The objective of this study is to examine a family of transmission boundary problems governed by second-order operational differential equations of elliptic type within the LP framework. The fundamental hypothesis, derived from the theory of sums of linear operators, is based on the theory of semigroups, interpolation spaces and certain results of Dore and Venni. This is employed to demonstrate the existence, uniqueness and maximum regularity of the strict solution to the posed problem.

Introduction

Let us consider, in the complex Banach space X, the following operational complete elliptic differential equation of the second order

$$\begin{cases} u_-''(x)+2Bu_-'(x)+Au_-(x)=g_-(x), & x\in(-\infty,0) \\ u_+''(x)+2Bu_+'(x)+Au_+(x)=g_+(x), & x\in(0,\delta) \\ (t.c)\begin{cases} u_-(0)=u_+(0) \\ \mu_-u_-'(0)=\mu_+u_+'(0)+\mu_-Hu_-(0) \end{cases} \\ (b.c)\begin{cases} u_+'(\delta)=f_+ \\ u_-(-\infty)=0 \end{cases} \end{cases} \qquad (1)$$

where A, B and H are closed linear operators in X. f_+ is a given element in X, μ_+,μ_- are two positive non-zero real constants expressing the conductivity of two bodies $(-\infty,0)$ and $(0,\delta)$. The second members

$$g=\begin{cases} g_-\in L^p(-\infty,0;X) \\ g_+\in L^p(0,\delta;X) \end{cases} \qquad with\ 1<p<+\infty$$

we search for a strict solution *u* to (1), i.e a function *u* such that:

$$\begin{cases} u_-'' & ,Bu_- & ,Au_-\in L^p(-\infty,0;X) \\ u_+'' & ,Bu_+' & ,Au_+\in L^p(0,\delta;X) \end{cases}$$

We decompose Problem (1) into two auxiliary problems (P_-) and (P_+). In order to solve Problem (1) for any $g_-\in L^p(-\infty,0;X)$, $g_+\in L^p(0,\delta;X)$ with $1<p<+\infty$. More generally, the problem posed becomes the following operational problem:

$$\begin{cases} u_-''(x)+(L-M)u_-'(x)-(LM)u_-(x)=g_-(x), & x\in(-\infty,0) \\ u_+''(x)+(L-M)u_+'(x)-(LM)u_+(x)=g_+(x), & x\in(0,\delta) \\ (t.c)\begin{cases} u_-(0)=u_+(0) \\ \mu_-u_-'(0)=\mu_+u_+'(0)+\mu_-Hu_-(0) \end{cases} \\ (b.c)\begin{cases} u_+'(\delta)=f_+ \\ u_-(-\infty)=0 \end{cases} \end{cases} \qquad (2)$$

Then, in order to resolve (1), we resolve (2). When L and M are some closed linear operators in X satisfying

$$\begin{cases} L - M \subset 2B \\ LM \subset -A \end{cases}$$

Where

$$L = Q + B \qquad M = Q - B \qquad Q = -\sqrt{B^2 - A}$$

we seek for a classical solution *u* to (2), so a function *u* such that

$$\begin{cases} u_-'' \ , (L-M)u_-' \ , (LM)u_- \in L^p(-\infty, 0; X) \\ u_+'' \ , (L-M)u_+' \ , (LM)u_+ \in L^p(0, \delta; X) \end{cases}$$

Theorem 1

based on a certain hypothesis that we used. Let $g_- \in L^p(-\infty, 0; X)$ and $g_+ \in L^p(0, \delta; X)$ with $p \in]1, +\infty[$. Then the problem in (2) has a unique strict solution u satisfying (2) that is

$$\begin{cases} u_- \in W^{2,p}(-\infty, 0; X) \cap L^p\big(-\infty, 0; D(LM)\big); \quad u_-' L^p\big(-\infty, 0; D(L-M)\big) \\ u_+ \in W^{2,p}(0, \delta; X) \cap L^p\big(0, \delta; D(LM)\big); \quad u_+' L^p\big(0, \delta; D(L-M)\big) \\ u_+(0) \in D(H) \end{cases}$$

if and only if

$$f_+ \in (D(LM); X)_{\frac{1}{2}+\frac{1}{2p}, p}$$

where f_+ is defined in the auxiliary problem (P_+).

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An easy enhancement in the efficiency of the Nguyen-Widrow initialization method in neural networks

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Abstract

The choice of the initial weights of the hidden layers of an aArtificial neural network (ANN) is a fundamental point for convergence within a reasonable time. In the early days of neural methods, researchers agreed that initial values can be generated by a Uniform law over a small interval centered on zero. Without prior information, this selection method does not necessarily lead to good training of the network. The final targeted parameter values may be very far from the initial values.

The goal of this work is to reveal the insidious reasons that cause unsuccessful attempts and prevent taking full advantage of the Nguyen-Widrow initialization method. Our analysis gives the preventive measures that would guarantee correct and permanent functioning of this method. These measures first eliminate situations that would lead to training failure. Determining the optimal number of hidden neurons is thus greatly facilitated and overfitting is more easily detected by this method.

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Asymptotic Normality of a Kernel Conditional Quantile Estimator

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Abstract

This paper aims at establishing the asymptotic normality for a kernel conditional quantile estimator in a right censorship model for which the lifetime observations and the covariates are assumed to satisfy an association dependency type.
KEYWORDS: Association, asymptotic normality, censored data, conditional quantile, Kaplan-Meier estimator.

1 Introduction

In classical statistical inference, the observed random variables (rv's) of interest are generally assumed to be independent and identically distributed (iid). However, it is more common to have dependent variables in some real-life situations. Dependent variables are present in several backgrounds such as medicine, biology, and social sciences. Associated rv's are of considerable interest when dealing with survival analysis, reliability problems, percolation theory, and some models in statistical mechanics.

In the literature, two kinds of dependency are widely used: mixing [DOUKHAN 1994] and association [ESARY et al. 1967]. These two concepts are not completely dissociated.

Recall that a set of finite family of rv's $(T_1, \ldots, T_n)$ which are defined on a common probability space $(\Omega, \mathcal{A}, P)$ are said to be associated if for every pair of non-decreasing componentwise functions $\varphi_1(\cdot)$ and $\varphi_2(\cdot)$ from $\mathbb{R}^n$ to $\mathbb{R}$,

$$\operatorname{cov}(\varphi_1(T_1, \ldots, T_n), \varphi_2(T_1, \ldots, T_n)) \geq 0,$$

whenever the covariance exists. An infinite family of rv's is associated if any finite sub-family is a set of associated rv's. The notion of association was first introduced by [ESARY et al. 1967] mainly for an application in reliability and its main advantage compared to mixing is that the conditions of limit theorems are easier to verify: indeed, a covariance is much easier to compute than a mixing coefficient.

Let $\{T_n, n \geq 1\}$ be a strictly stationary sequence of associated rv's of interest having an unknown absolutely continuous distribution function (df) F.This variable can be considered as a lifetime in biomedical studies, characterized by incompleteness due to random right censoring. This means that the available data provide only partial information, as the duration is censored when a specific event occurs, such as the patient remaining alive or dying for other reasons. In this case, the variable of interest T is subject to right censoring by another non-negative rv C. We assume that the censoring lifetimes are independent and identically distributed (iid) with an unknown distribution function G. Additionally, we consider a strictly stationary and associated covariate X taking values in $\mathbb{R}^d$. The observable sequence is defined as: $\{(Y_i = \min(T_i, C_i), \delta_i = 1_{\{T_i \leq C_i\}}, X_i) : 1 \leq i \leq n\}$, where the indicator function 1_A denotes the event A. To ensure model identifiability, we assume that the censoring times $\{C_i\}$ are independent of the pairs $\{(X_i, T_i)\}$. Under this framework, the asymptotic normality of the kernel conditional quantile estimator is established.The rest of the paper is organized as follows: Section 1 gives the required notations as well as the estimators. The assumptions needed to state our results are gathered in Section 2 while Section 3 is devoted to the proofs of the main results.

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Solving the Diophantine Equation $F_n^{(k)} L_m^{(k)} = \dfrac{a(10^\ell - 1)}{9}$

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Abstract

For an integer $k \geq 2$, let $(F_n^{(k)})_{n \geq -(k-2)}$, $(L_n^{(k)})_{n \geq -(k-2)}$ be the k-Fibonacci and the k-Lucas sequences, respectively. For these sequences the first k terms are $0, \ldots, 0, 1$ and $0, \ldots, 0, 2, 1$, respectively, and each term afterwards is the sum of the preceding k terms.

A positive integer is called a repdigit if it has only one distinct digit in its decimal expansion. In particular, such number has the form $a(10^\ell - 1)/9$, for some $l \geq 1$ and $1 \leq a \leq 9$.

Several problems involving generalized Fibonacci sequences or generalized Lucas sequences and repdigits have been of interest to mathematicians. For instance, Luca and Marques proved that 55 and 44 are the largest repdigits in the sequences $F^{(2)}$ and $F^{(3)}$, respectively. Moreover, Luca showed that 11 is the largest repdigits in the sequences $L^{(2)}$. Recently, Erduvan and Keskin have studied repdigits as product of two Fibonacci and two Lucas numbers. Motivated by these results, we will study the solutions of the Diophantine equation

$$F_n^{(k)} L_m^{(k)} = \frac{a(10^\ell - 1)}{9}. \tag{0.1}$$

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Bayesian and Non-Bayesian Analysis of the New One-Parameter Model under Right Censored Data

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Abstract

We propose a one-parameter of inverse Gompertz distribution (DGI) for right censored Bayesian and non-Bayesian. The parameter of this distribution is estimated using several conventional methods, including the Bayesian method.
The likelihood and Bayesian estimates are compared using Pitman's closeness criteria. The Bayesian estimators are derived using three loss functions: the extended quadratic, the Linex, and the entropy functions.
All the estimating approaches offered have been assessed through simulated experiments. Real data applications are considered in the performance of the DGI model. The censored maximum likelihood method and the Bayesian approach are compared using the BB algorithm.

Keywords: inverse Gompertz distribution; Bayesian estimation; BB algorithm; censored data; Pitman's proximity.

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Probability of Failure of a Corroded Pipeline Considering Correlations Between Random Variables

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Abstract

Transporting hydrocarbons via pipelines is still regarded as the most economical and widely used method [1]. To ensure the safety of this transport method, several precautions have been implemented, including internal coatings, external coatings, and cathodic protection, in response to numerous challenges, with corrosion being a primary cause of the degradation of mechanical properties and toughness in steel pipelines. On production sites, pipeline lifespan is primarily tied to general corrosion, which accounts for 25% of failures in steel gas pipelines and over 60% for metallic structures [2]. Buried pipelines are expected to withstand external stresses, particularly the aggressive environment and pressures caused by the transported fluid. Localized corrosion is the most dangerous form for buried steel pipelines, making its consideration essential during analysis [3]. Addressing uncertainties in the random variables of both the resistance and load in the performance function is critical for making the analysis more realistic. Thus, unlike deterministic approaches, probabilistic approaches offer better answers for maintenance and design, serving as a decision-making tool for potential repairs or replacements of damaged pipeline sections [4].

Keywords: Reliability, Random variables, correlation, corrosion defect

Results and Discussion

The results of the reliability analysis based on the DNV-RP-F101 standard as a function of defect length L for different ratios of defect depth to pipe thickness, d/t. Based on pipeline inspection data and to guide the investigation, five ratios were chosen : 25%, 35%, 55%, and 65%. The reliability index decreases as the defect length increases for all corrosion defect depths. Higher defect depth-to-thickness ratios are more sensitive to defect length compared to lower ratios. Damage tolerance suggests that for deeper defects, shorter defect lengths are acceptable for damaged pipeline sections, based on the reliability index. It is also crucial to estimate the impact of gas pumping duration on the degradation of pipeline reliability for each damaged segment. Modeling this behavior can serve as a decision-making tool for maintenance or the replacement of damaged pipeline sections. The effect of pipeline service time on the degradation of the reliability index β as a function of defect length for each corrosion defect depth. As expected, for deeper defects, the damage tolerance in terms of defect length is reduced compared to shallower defects. This is due to the significant variation in the corrosion propagation rate, assuming that this rate remains uniform throughout the entire service life of

the pipeline. This trend highlights the increasing impact of deeper defects on structural degradation, thereby reducing the safety margin over time.

It is well understood that the degradation of pipeline reliability increases with higher service pressure. This degradation is more pronounced for the largest corrosion defect ratios. The increase in service pressure from 70 bars to 100 bars leads to a significant drop in the reliability index, highlighting the importance of plotting a contour diagram based on the modelled results of the reliability index in relation to service pressure and defect length. A decision-making tool for a maintenance program is developed, illustrating contour diagrams of the reliability of corroded API 5L pipelines as shown in **Fig. 1**. The scatter plot section of the diagram represents the domain where the pipelines are safe, with no risk to production. In the second part of the diagram, delineated by the target contour β=3.72 (white zone), a maintenance plan should be anticipated.

The sensitivity of the variables in the developed mechanical model. The three key variables namely pressure, ultimate stress, and thickness are the most important in the mechanical model. The tube thickness exhibits an almost constant sensitivity and is not affected by pressure variations, while the other two variables are highly sensitive, resulting in a competition between their sensitivities.

Conclusions

The developed probabilistic approach is used to investigate the effect of localized corrosion on the lifespan of high-yield strength pipelines. The mechanical model used for assessing corrosion defects is based on the DNV-RP-101 standard. Based on the inspection results of buried pipeline defects intended for gas transport over three decades, their lifespan is estimated according to the ratio of defect depth to pipe thickness, defect length, and the service pressure of the fluid being transported. A failure probability diagram is developed for the damaged pipeline. The sensitivity analysis results show that the combination of the service pressure of the fluid being transported, the ultimate stress of the material, and the pipe thickness are the most dominant factors affecting the reliability of the API 5L pipelines. Therefore, strict control of gas pressure fluctuations is essential for managing the probability of failure in damaged pipelines.

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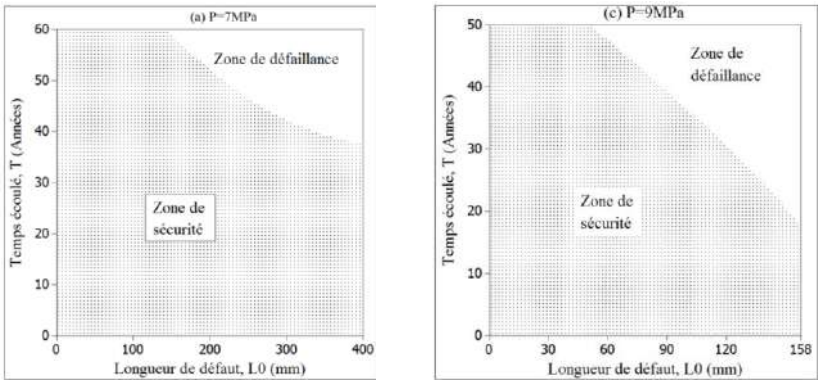


Fig.1. Reliability diagram for the damaged pipeline section with a ratio *d0/t*=25% (a) P=7 MP, and (b) *P*=9 MPa.