Book of Abstract

NCTPA 2025

11th National Conference on Theoretical Physics and Applications

December 1st-3rd 2025

Edited by:

N. Bouchemla, N. Laouet, L. Ghegal and H. Naidja

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Foreword

It is a great pleasure to open this 11th edition of theoretical Physics and applications conference (NCTPA) here in Constantine, Algeria, at Constantine 1 university.

The National Conference on Theoretical Physics and its Applications (NCTPA'25), organized by the Laboratory of Mathematical physics and subatomic physics (LPMPS), took place at Frères Mentouri Constantine 1 University from December 1-3, 2025. This event marks the eleventh edition of a distinguished series of national conferences that began in 1992, under the initiative of the late Professor Nouredine Mebarki. The (NCTPA'25) was designed to bring together researchers from across Algeria working in various areas of theoretical and applied physics. It aimed to create a welcoming and inspiring environment for scientific dialogue, where Algerian scientists and researchers could exchange ideas, share their latest findings, and strengthen collaborations across disciplines. The conference covered a wide range of topics:

- Mathematical physics and applications
- Standard model and beyond
- Gravitation and quantum cosmology
- Quantum information
- Nuclear physics and applications
- Theoretical chemistry and applications
- Artificial intelligence in physics.

127 abstracts were received covering all the fields reviewed by the organizing Committee, scheduled on plenary, parallel and posters sessions.

On behalf of the Organizing Committee, we would like to express our sincere gratitude to all participants from different Algerian universities for their valuable scientific contributions to the success of the NCTPA'25. We also extend our heartfelt thanks to the organizing team for their dedication, effort, and commitment that made this event possible.

We wish you a successful and fruitful conference and pleasant stay in Constantine.

About LPMPS

The Laboratory of Mathematical Physics and Subatomic Physics (LPMPS) is one of the most renowned research laboratories in Algeria in the field of theoretical physics. Founded in 2000 and located at the Frères Mentouri Constantine 1 University, the laboratory brings together a large team of dedicated teacher-researchers, led over the years by a succession of eminent Algerian physicists.

The Laboratory of Mathematical and Subatomic Physics (LPMPS) is one of Algeria's most renowned research laboratories in the field of theoretical physics. Founded in 2000 and located at Frères Mentouri University Constantine 1, the laboratory brings together a large team of dedicated teacher-researchers, led over the years by a succession of eminent Algerian physicists.

LPMPS has been recognized several times as a "Center of Excellence" and continues to play a leading role in physics research, both nationally and internationally. His work covers a wide range of fields, including:

- Mathematical physics
- High-energy physics and gravitation
- Quantum computing and field theory
- Nuclear physics and radiation-matter interaction
- Medical and applied physics
- Computational and theoretical chemistry

LPMPS is also committed to training future physicists through research-oriented teaching, thus ensuring students receive a solid foundation in fundamental physics and related disciplines. Many of its graduates have subsequently made significant contributions to academia, research, and industry.

Scientific Leadership at LPMPS Over the Years:

- Prof. Lyazid Chetouani (2000–2005): Founding Director, played a pivotal role in defining the laboratory's initial vision and direction.
- Prof. Nouredine Mebarki. (2005–2021): Founding member and highly respected physicist, remembered for his exceptional contributions and leadership until his death from COVID-19.
- Prof. Aissaoui Habib (2021–2023)
- Prof. Houda Naidja (2023–present)

Research Teams at LPMPS:

LPMPS is organized into specialized research teams , each focused on key areas of theoretical and applied physics:

- **Team 1**: Mathematical Physics, High Energy Physics, Gravitation, and Quantum Computing;
- **Team 2**: Strings, Gravitation, and Quantum Information;
- **Team 3**: Nuclear Physics and Radiation-Matter Interaction;
- **Team 4**: Path Integrals and Quantum Processes;
- **Team 5**: Radiation-Matter Interaction and Applications;
- **Team 6**: Synthesis and Study of the Physicochemical Properties of Carbon Nanoparticles;
- **Team 7**: Nuclear Structure and Applications;
- **Team 8**: Computational and Theoretical Chemistry

LOCAL SCIENTIFIC COMMITTEE

Chair: Prof. Houda Naidja

Prof. Aissaoui Habib	Prof. Bentag Baya
Prof. Belaloui Nadir	Prof. Mimouni Jamel
Prof. Ait Moussa Karim	Prof. Bensouici Aicha
Prof. Benabbes Ouenassa	Prof. Labani Rebiha
Prof. Benrachi fatima	Prof. Belkhiri Lotfi
Prof. Benslama Achour	Prof. Benhizia Karima

Plenary Sessions

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Quantum computing with mechanical oscillators

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Quantum computers are systems capable of performing computations by exploiting the laws of quantum physics. Quantum computers can be realised on many platforms, such as levitated atoms, superconducting circuits, and photons. Information is encoded in the quantum state of the system, and the computation is performed via the application of operations on the system, leading to its state being changed—i.e. the processing of information. Quantum computation can be implemented as the evolution operator of the system, where the outcome of the computation will be the final state of the system. Equivalently, the computation can also be implemented by preparing an entangled state of the system, called a cluster state, and then measuring a set of observables; the outcome of computation will be encoded in the post-measurement state. This latter approach to quantum computing is known as measurement-based quantum computation.
In this talk, I will talk about measurement-based quantum computation using mechanical oscillators as carriers of information. More specifically, I will show how to prepare a cluster state of many mechanical oscillators with the help of an optomechanical system. Then, I will discuss how to perform measurements on the system in order to implement arbitrary unitary operations, thereby enabling universal quantum computation.

Keywords:
Cluster states; Quantum optomechanics; Quantum computation over continuous variables; measurement-based quantum computation.

Sadouni Salheddine

Intelligence Artificielle : Nouveaux Outils au Service de la Recherche Scientifique

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La recherche scientifique constitue aujourd'hui un levier essentiel du développement socio-économique, de l'innovation et de la compétitivité des nations. Dans un contexte mondial marqué par l'accélération de la production scientifique et l'évolution rapide des technologies, les jeunes chercheurs sont appelés à exploiter pleinement les outils numériques et méthodologiques mis à leur disposition. Parmi ces outils, l'Intelligence Artificielle occupe une place centrale, offrant de nouvelles perspectives pour améliorer la qualité des travaux, optimiser les processus de recherche et accélérer la production scientifique.

Cette présentation mettra en lumière les nouveaux outils d'IA dédiés à l'optimisation du travail scientifique. Elle abordera notamment les solutions permettant d'améliorer la rédaction académique, la révision linguistique, l'analyse bibliographique, la gestion des références, la détection de similarités, ainsi que les outils d'aide structurelle à la préparation des articles et rapports de recherche. L'accent sera également mis sur les plateformes d'IA capables de soutenir les chercheurs dans la préparation, la soumission et la diffusion de publications scientifiques de haute qualité.

En offrant un panorama complet et pratique de ces technologies émergentes, cette intervention vise à sensibiliser et à accompagner les jeunes chercheurs dans l'intégration efficace de l'IA au cœur de leur démarche scientifique, afin d'accroître la pertinence, la visibilité et l'impact de leurs travaux.

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Conformal Killing Gravity; Another theory of gravity

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This talk presents a new theory of gravity, referred to as Conformal Killing Gravity, which is a third-order extension of general relativity. We explore its solutions and geometrical properties in spherically symmetric spacetimes with Maxwell fields. These solutions, characterized by six independent parameters, encompass non-asymptotically flat black holes and naked singularities, as well as non asymptotically flat traversable wormholes and (potentially singularity-free) closed universes. Additionally, we investigate sourceless, time-dependent solutions in FRW spacetimes. These solutions, depending on the spatial curvature, the cosmological constant, and a novel integration constant α, exhibit a rich variety of cosmological behaviors. These include singularity-free eternal cosmologies and symmetric universes evolving from a big bang to a big crunch within a finite time span. We finally discuss potential limitations and challenges faced by the theory.

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Nuclear physics applications

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Nuclear physics, which studies the structure and dynamic of the atomic nucleus, has given rise to numerous beneficial applications in several key sectors of modern society.

1. Energy production

One of the main applications of nuclear physics is the production of electrical energy in nuclear power plants. The principle is based on nuclear fission, where a heavy nuclei (such as uranium-235 or plutonium-239) are split into lighter nuclei, releasing a large amount of energy in the form of heat. This heat is used to produce steam, which drives turbines connected to alternators. Nuclear energy has the advantage of high energy density and low greenhouse gas emissions, although radioactive waste management and reactor safety remain major challenges. Current research is also focused on nuclear fusion, a potentially inexhaustible and cleaner source of energy.

2. Nuclear medicine

In medicine, nuclear physics plays an essential role in diagnosis and treatment. Radioisotopes (such as technetium-99m, iodine-131, and fluorine-18) are used to visualize organ function through scintigraphy and positron emission tomography (PET). These techniques can detect tumors, heart disease, and metabolic disorders. In terms of treatment, radiation therapy uses ionizing radiation (gamma, beta, neutron or proton) to selectively destroy cancer cells while preserving healthy tissue as much as possible.

3. Industry:

In industry, nuclear physics has many applications. Radioactive sources are used for non-destructive testing (industrial radiography) to inspect the quality of welds, metal parts, or structures without damaging them. Radioactive tracers are used to analyze fluid flows in pipelines or chemical processes. Neutron counters and radiation gauges are also used to measure the density, thickness, or level of materials in manufacturing processes. These techniques increase the safety, accuracy, and profitability of industrial processes.

4. Agri-food:

In the agri-food sector, nuclear physics contributes to improving food production and preservation. Radioactive sterilization or food irradiation eliminates microorganisms, parasites, and insects, extending the shelf life of products without the use of chemical additives. Stable and radioactive isotopes are also used to study soil fertilization, plant metabolism, and food traceability. These applications promote more sustainable agriculture and better food safety.

In conclusion, nuclear physics, although often associated with risks, is an essential pillar of scientific and technological progress. Its applications in energy, health, industry, and agri-food demonstrate its potential to improve quality of life while posing ethical and environmental challenges that must be addressed.

Key words :

Nuclear reactions, nuclear reactors, nuclear medicine, radiation-therapy, Nuclear techniques analysis, neutrons sources applications.

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Theoretical investigation of the electronic structure and magnetic properties of single-atom bridged diuranium UXU (UIII/IV/V; X = N_{3-}, O_{2-}, S_{2-}) complexes.

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Electronic structure and magnetic properties of single-atom bridged Aryl diuranium [(U(OAr)3)2(μ-X)]q (UIII/IV/V; X = N3-, O2-, S2- ; q = −3, −2, −1, 0 ; OAr = 2,6-di-tert-butylphenoxide) complexes, exhibiting diverse magnetic U—X—U exchange coupling, have been investigated computationally using scalar relativistic density functional theory combined with the broken symmetry (BS) approach. These complexes include nitride U—N—U [(U(OAr)3)2(μ-N)]q species, oxide U—O—U [(U(OAr)3)2(μ-O)]q, and their sulfide U—S—U [(U(OAr)3)2(μ-S)]q congener, exhibiting trivalent UIII/UIII state, tetravalent UIV/UIV, and mixed-valence UIII/UIV, UIV/UV derivatives. The calculated coupling constants JU-U agree with the observed antiferromagnetic character observed in the case of the UIV/UIV [(U(OAr)3)2(μ-N)]- and the UIII/UIII [(U(OAr)3)2(μ-O)]2- complexes. The structural parameters, in particular the U—X distances and the U—O—U angles, as well as the electronic factors driving the super-exchange couplings, are discussed. The Mayer and Nalewajski/Mrozek (NM) bond orders and the magnetic molecular orbital analyses reveal that the U(5f)—O(2p)—U(5f) covalent contribution to the bonding within the U—X—U coordination is more important in the nitride U—N—U species complexes than in the oxide U—O—U and sulphide U—S—U congeners, thus favouring AF coupling between the two uranium magnetic centers. The Natural Populations Analyses confirm the crucial role of spin delocalization that is at work in favour of the AF vs. Ferromagnetic character of the U—X—U coordination.

Keywords:

diuranium U—O—U complexes; magneto-structural correlations; super-exchange; ZORA/DFT, Broken Symmetry.

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Parallel Sessions

Nuclear Physics and Applications

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Revealing Trends in the ^{132}Sn Region Using Particle-Hole Derived Effective Interaction

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Understanding nuclear structure of systems far from stability is essential for elucidating the spectroscopic properties of nuclei. In this work, we develop a new effective interaction using the low-momentum potential approach to study nuclei near ^{132}Sn, specifically those containing neutron holes. This presentation will focus on the energy levels of nuclei in the range of $Z \geq 50$ and $N \leq 82$, as well as magnetic dipole moments and first excited-state electric transitions, compared to existing experimental data.

Keywords:
Effective interactions, shell-model, spectroscopy, Antoine

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Low-Lying Structure of N=50 Isotones with Residual Vlow interaction

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The N=50 isotones, in the vicinity of ^{78}Ni doubly magic serve as a critical testing ground for the stability of the Z=28 proton shell closure and the evolution of proton single particle energies in the $fpg_{9/2}$ shells. Studying the low-lying structure of these nuclei is essential for refining the effective nuclear interaction used in the modern shell model calculations. The current study aims to investigate the low-lying excitation spectra and electromagnetic properties of the N=50 isotones of even and odd-A, using the residual interaction derived from the Kuo-Lee-Ratcliff (KLR) folder diagram expansion in terms of the vertex function Q box called Vlow . calculations was performed with NuShellX@MSU shell model code, considering the ^{56}Ni as inert core and the model space is ($1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$ and $1g_{9/2}$) for both protons and neutrons. Our results indicate that the used interaction successfully reproduce the general trend of the first excited state for the studied nuclei. Also it shows good agreement with the available experimental spectra

Keywords:
Shell model, N=50 isotones, Vlow interaction

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Microscopic description of neutron-rich nuclei around ^{90}Zr

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The aim of the present work is to study the spectroscopic properties of isotonic chain N=50 with Z>40. The calculations are achieved by using a new effective interaction developed for this mass region within the framework of perturbation theory.
Using a new effective interaction developed by low-momentum potential approach to present the energy levels of a chain of nuclei around ^{90}Zr with N=50 and Z>40.
The calculations were performed within the shell model framework [2], and the numerical calculations were carried out using Antoine shell-model code [2,3].
The calculated energy levels of the N=50 isotonic chain with Z>40 are in good agreement with the experimental data. This confirms the validity of the neutron-neutron matrix elements part of our new effective interaction.
Conclusion/Implications: The results will be extensively discussed, with the prediction of new ones not yet experimentally observed.

Keywords:
Shell model, nuclear structure, effective interaction.

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Assessment of radiological biological risks in environmental samples

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Radioactive substances are naturally present in the environment and can also originate from human activities. These radionuclides may pose risks to human health and ecosystems, making it important to assess their presence and impact. In this study, gamma spectrometry was used to measure the activity concentrations of natural radionuclides in environmental samples. Based on these measurements, radiological hazard indices such as the absorbed dose rate and hazard indices were calculated. The results were compared to safety limits recommended by the United Nations Scientific Committee on the Effects of Atomic Radiation (UNSCEAR). The findings show that radioactivity levels in the samples are generally within safe limits, indicating low risk from both external and internal exposure. This study contributes to understanding the radiological safety of the environment and supports ongoing monitoring and risk management efforts.

Keywords:
Radiological risk, Gamma spectrometry, Radionuclides, Environmental samples

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Commissioning data of flattening filter free (FFF) photon beams

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Various cancer centers in Algeria have been prepared to use flat filter-free (FFF) photon beams generated by medical linear accelerators in radiotherapy but the basic dosimetric data acquisition accuracy is crucial for using this beam type because it directly correlates to the dose given to patients. This study aims to present, analyze, and evaluate the data collected from FFF photon beam commissioning.
Basic dosimetric data have been analyzed and compared, they are generated by a Varian medical linear accelerator "True beam", having both FFF and flat beams (FF) of 6 and 10 MV energy, these data are measured according to the TPS "Eclipse" commissioning recommendations. The evaluation entails absorbed dose rate in water, beam quality, percentage depth dose (PDD), lateral dose profiles and collimator output factor in free field for various field sizes and depths.
The analysis of the PDDs reveals that the difference increases with depth. The maximum dose has a difference of around 1mm. In small fields, the skin dose of the FFF beam is higher, but it becomes similar in large fields. The profile shape stays the same from the smallest fields to 10x10cm², but there is a significant change in the profile shape when the field size increases. The output factor is higher for small fields, but lower for large fields. FFF beams have a lower output factor value variation between the smallest and largest fields, unlike FF beams. The FFF beam's beam quality was found to be less than that of the FF beams with an acceptable reference dose rate difference of 0.1 cGy/MU. The evaluated data was fully consistent with the different publications.
This study provided us with valuable information about the properties of FFF beams, their differences compared to flat beams, and their consistency. It also indicates the reliability of our measurements.

Keywords: Flattening Filter Free (FFF), High dose rate, Dosimetric data, commissioning.

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A=105 β decay properties

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Proton rich unstable nuclei have received increasing interest in recent nuclear structure studies. These exotic systems facilitate the advancement of theoretical modelling focused on nuclear structure. In this context, the work carried out within the framework of this study is based on the nuclear structure and Gamow-Teller decay calculations of A=105 isobars close to the astrophysical rp-process path. The calculations are carried out in the framework of nuclear shell model, by means of NushellX@msu nuclear structure code. Using CD-Bonn [4] original interaction, we have realised some modifications, based on the monopole effect, to introduce new effective one. The calculated nuclear structure and beta decay properties are then compared to the available data, in order to emphasise the role of the considered effect and to improve the available nuclear potentials.

Keywords:
Nuclear structure, Beta decay, ^{100}Sn doubly magic core, Monopole interaction

References:

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High Spin Bands Interpretations of Odd Cerium Isotopes

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The Cranked *Nilsson Strutinsky* (CNS) model is applied to study odd cerium isotopes. Total energies are calculated and compared with observed values. Divers configurations are assigned to interpret the different bands. The shape evolution is determined in function of deformation parameter ($\varepsilon 2$, γ) and of the kinematic $J^{(1)}$ and dynamic $J^{(2)}$ momentum of inertia values.

Keywords:
Cerium isotopes, Cranking Nilsson Strutinsky (CNS), Shape evolution and Deformation parameters.

References:

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Three-Body Correlations in the Hydrodynamic Description of Quantum Mixtures

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In this work, we investigate the role of three-body interactions within the hydrodynamic description of quantum mixtures, in the presence of strong interaction systems. The mixture. Starting from the interconnected hydrodynamic equations, where analytical and numerical results reveal that these higher-order correlations significantly affect both the stability of the system and its dynamic behavior, we also provide a deeper insight into the complex interaction between multiparticle interactions and hydrodynamic responses in ultracold quantum mixtures and compare our results with other studies.

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Study of valence multi-hole nuclei near the heaviest doubly magic nucleus

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Theoretical and experimental study of nuclei far from the stability is an important subject in nuclear Physics and astrophysics also. The information about excitation energies and nucleon-nucleon interaction obtained in each part of nuclear chart can be tested the basic ingredient of shell model calculation. This work aims to investigate the even $^{206-194}$Pb isotopes in ^{208}Pb mass region with khhe interaction [1,2] of the code library and single particle energies [3].The calculation are performed in the frame work of the nuclear shell model by means of NuShellX@MSU code[4]. The results are then compared to the available experimental data.

Keywords: Shell model, khhe interaction, NuShellX code, model space jj56pn.

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Comparative Analysis of External Radiotherapy Techniques for the Treatment of Head and Neck Cancers

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Background/Introduction:
External beam radiotherapy treatment for head and neck cancers is very complex due to the complex anatomical structure of this region. Many radiotherapy techniques are used to precisely treat these cancerous locations, such as the five-field conformal technique and the VMAT technique. However, several questions arise: Which technique offers the patient precise treatment and a better quality of life? Which technique provides the best coverage, conformity, and dose homogeneity? And which technique minimizes the toxicity at the level of the osteoarticular receptors (OARs) and thus the adverse effects of external beam radiotherapy?

Objective:
Three-dimensional conformal radiotherapy (3D-CRT) remains the conventional five-field technique for the treatment of head-and-neck malignancies and has been established as a reference standard for organ-at-risk (OAR) preservation, target coverage, and dose conformity for many years. With the emergence of advanced techniques such as Volumetric Modulated Arc Therapy (VMAT), a comparative assessment is justified to delineate the respective strengths and limitations of each modality.

Methods:
Ten patients diagnosed with nasopharyngeal carcinoma were retrospectively selected from the ATHENA Medical Center database. For each patient, treatment plans using 3D-CRT and VMAT were generated. Plan comparison was performed with respect of dose coverage and toxicity, dose homogeneity index (HI), conformity index (CI), and quality index (QI).

Results:
VMAT provided superior sparing of the parotid glands, total optics, and brainstem while maintaining adequate coverage of the target volumes. The two techniques have clearly different values for all evaluated indices (TC, CI, HI, and QI).

Conclusion/Implications:
The VMAT technique increases thecompliance index and the minimum dose for the target volumes compared to 3D -CRT in patients with oropharyngeal cancer. It has also led to a decrease in maximal brainstem dose and total optics,as it protects a large part of the parotid glands..

Keywords: 3D-CRT, VMAT, Head-and-Neck Cancer, Nasopharynx, Dosimetric Evaluation.

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Quantum Information

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Thermodynamics of Massless Pair Creation Fermionic Modes in Deformed Spacetime

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A deformed Dirac equation and its solutions are derived. Our results show that the space-time noncommutativity contributes to the creation of entangled particle. Using the von Neumann entropy, as well as the Bogoliubov transformations technique, we quantify the created quantum entanglement between massless fermionic modes in noncommutative 2D De Sitter spacetime. Our research show that the behavior of quantum entanglement is strongly affected by some parameters, the noncommutativity (N.C.) θ parameter, the k-frequency modes as well as the structure of the spacetime. According to our numerical results, we notice that the structure and deformation of the space–time as well as the type of the involved particles (fermions or bosons) affect the behavior of quantum entanglement. Our results show that we can use quantum entanglement to determin some of the thermodynamical properties of the spacetime.

Keywords:
Quantum entanglement, von Neumann entropy, noncommutative θ parameter, Chemical potential.

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TQSim: a Library for Systematic Computation of Braid Generator Matrix in Topological Quantum Computation

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Topological Quantum Computation (TQC) provides an inherently fault-tolerant paradigm for quantum information processing by encoding quantum information in non-Abelian anyons and performing logic through their braiding. While the theoretical formalism for constructing braid group representations from the fusion and rotation (F and R) matrices of a given anyon model is well established, a systematic numerical method and software implementation capable of handling complex fusion spaces and large anyon systems has remained absent. This work introduces TQSim, a comprehensive computational library developed to systematically generate and simulate braid generator matrices for arbitrary anyon models. The objective is to provide a numerically stable, and model-agnostic framework for constructing elementary braid operations and simulating topological quantum circuits. TQSim implements a novel algorithm for braid computation which is based on a "knitting" move, enables efficient generation of braid matrices within a sparse encoding scheme, accommodating arbitrary numbers of anyons per qudit. The method is integrated into a modular Python-based architecture, supporting symbolic and numerical computation, fusion tree manipulation, and circuit-level simulation. The library successfully reproduces known braid matrices for standard anyon models and demonstrates its enhanced scalability by simulating an approximated CNOT gate and a five-qubit GHZ state encoded using three Fibonacci anyons per qubit—representing the first numerical realization of such a system. These results validate TQSim's capability to handle complex multi-qubit topological circuits and confirm its accuracy in reproducing expected topological gate operations. TQSim provides the first systematic and general-purpose numerical framework for braid matrix computation in TQC. By enabling efficient exploration of arbitrary anyon models and circuit constructions, TQSim lays the groundwork for future studies on topological gate synthesis, algorithm design, and fault-tolerant quantum architectures.

Keywords: Topological quantum computation, anyons, braid matrices, quantum simulation, anyon models

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Quantum Simulation of the Unruh Temperature via the Thermal Properties of Virtually Evolving Bose-Einstein Condensates

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This paper presents a novel theoretical model motivate a new experimental scheme to simulate the Unruh temperature by relating it to the critical temperature of multiple Bose-Einstein thermal baths. These thermal baths are conceptualized as snapshots of a Bose-Firework originating from an evolving driven Bose-Einstein condensate (BEC). The critical temperature of each snapshot is determined from the heat capacity, which is numerically estimated by calculating the partition function derived from the system's Hamiltonian. By analyzing the relationship between the average number of the phononic excitations at the critical temperature, acceleration, and the critical temperature itself, our model demonstrates a significant agreement with the Unruh temperature formula, thereby validating our hypothesis. This theoretical approach offers a cost-effective alternative experimental setup compared to other resources-intensive experimental simulations. Furthermore, it provides a unique perspective on quantum simulation by utilizing the critical phenomena of condensed matter systems to probe fundamental quantum relativistic effects.

Background/Introduction:

This research investigates the theoretical correspondence between the Unruh temperature a relativistic thermal effect experienced by accelerated observers and the critical temperature of finite-size Bose-Einstein condensates, aiming to model this connection through a proof-of-concept quantum simulation framework. The study provides new insight into how phase transition phenomena in condensed-matter systems can serve as analogs for relativistic quantum effects, offering a cost-effective pathway toward future experimental realizations.

Objective:

The aim of this study is to establish a theoretical correspondence between the critical temperature of a Bose–Einstein condensate and the Unruh temperature, demonstrating how phase transition behavior can model relativistic thermal effects.

Methods:

The study employs a theoretical and numerical approach based on the Hamiltonian model inspired by a driven Bose–Einstein condensate experiment. Using exact diagonalization, the eigenspectrum of the system is computed to estimate the partition function, heat capacity, and critical temperature, which are then compared with existing experimental data from Hu et al. (2019) to validate the proposed correspondence with the Unruh temperature.

Results:

The results show that the critical temperature obtained from the thermal properties of the modeled

Bose–Einstein condensate closely mirrors the behavior expected from the Unruh temperature, confirming a consistent theoretical link between relativistic thermality and phase transition phenomena. This finding supports the feasibility of simulating relativistic effects using condensed-matter systems and provides a foundation for future experimental realizations.

Conclusion/Implications:

The study establishes a clear theoretical link between the critical temperature of a Bose-Einstein condensate and the Unruh temperature, offering a foundation for future analog quantum simulations of relativistic effects.

Keywords:

Unruh Temperature, Critical Temperature, Quantum Simulation.

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Simulations of molecular excited-State with Hybrid Quantum Algorithms: VQD vs VQE-AC

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The accurate simulation of molecular systems for solving electronic structure and energy spectra problems is challenging, especially for large molecules, as they involve multiple electrons and molecular orbitals, for which the Hilbert space scales exponentially with system size. Quantum computing offers a fundamentally new approach for tackling these problems by encoding the molecular Hamiltonian into qubits. It thus becomes possible to simulate the quantum evolution of the system and extract eigenvalues corresponding to ground- and excited-state energies more efficiently. In the pursuit of solving the multi-level electronic problem, our work implements and compares two hybrid quantum-classical methods, namely the Variational Quantum Deflation (VQD) and the VQE with Automatically-Adjusted Constraints (VQE-AC) algorithms. We show that the VQD, although simple to implement, can be inaccurate due to including the state orthogonality condition within the cost function. Alternatively, in the VQE-AC this condition becomes an external constraint to the quantum optimization routine, which renders this algorithm more accurate. We find that the VQE-AC is better in dealing with local minima issues, although at the cost of a more complex variational procedure.

Keywords:

Quantum Simulation, Variation Quantum Algorithm, Quantum Chemistry

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Mathematical Physics

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Extended NU-Method for Inverse Square Root and PDM Kratzer Potentials

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In this work, we apply the extended NU-method to two non-trivial quantum systems: (i) the inverse square root potential with constant mass, and (ii) the generalized Kratzer potential with position-dependent mass (PDM). The latter case requires a careful treatment of the kinetic energy operator, for which we adopt the general effective Hamiltonian first proposed by Von Roos [4]. To handle the centrifugal term, the Greene–Aldrich approximation [5] is employed, allowing us to derive closed-form expressions for the corresponding energy spectra. As a main outcome, we explicitly determine the energy eigenvalues for both systems.

Keywords:
NU-method, inverse square root potential, Kratzer potential with PDM, energy spectra

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Bosonic and Fermionic Strings with Modified Energy-Momentum Relations: Classical and Quantum

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This subject deals with analyzing bosonic and fermionic string models under modified relativistic energy-momentum relations. The research tries to explore the relationship between these modifications and Hamiltonian constraints, their algebras, and uses the canonical quantization method to give string energy spectra with new properties. This topic tries to study the interplay between classical dynamics and quantum behavior using the Hamiltonian approach, which clearly relates the Virasoro conditions to two-dimensional reparametrization invariance and deeply exhibits their character.

The importance of this subject lies in its potential to improve our understanding of the effect of energy levels on string theory symmetries. It can potentially shed light on the applications of such models in supersymmetry and quantum gravity, bridging the gap between classical and quantum properties.

Keywords:
Bosonic string, Fermionic string, energy-momentum relations.

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Open Fermionic Strings in Quantum Geometry: Effects of Non-Commutativity

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We explore the behavior of open fermionic strings in a non-commutative target phase-space, where the non-commutativity arises from an antisymmetric background field $B\mu\nu$. Starting from a deformed worldsheet structure described through the Moyal star product, the study reformulates the canonical commutation relations between coordinates and momenta. This deformation modifies the oscillato ralgebra and consequently alters both the super-Virasoro and Lorentz algebras, introducing θ-dependent corrections. Despite these modifications, the GSO projection ensures the physical consistency of the spectrum by removing tachyonic and unphysical lstates. The resulting mass spectrum exhibits non-trivial dependence on the non-commutativity parameters while preserving supersymmetry and conformalin variance. Physically, this analysis shows that the presence of the BBB-field transforms the target space time into a quantum geometry, where non-commutativity becomes anintrinsic feature without violating the fundamental symmetries of string theory.

Keywords:
Noncommutativephase-space, Super-Virasoroalgebra, Lorentzalgebra, GSO projection

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Generalized quantum mechanics and its effects

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In this work, we have studied some effect of q-deformation of momentum operator which leads to a GUP with minimal uncertainties in both of position and momentum measurements. Also, this q-deformation leads to non-hermitian operators. It has been explicitly shown that the harmonic oscillator Hamiltonian is pseudo-hermitian. The reality of the Hamiltonian eigenvalues has been illustrated by analytically computing the first order correction to the energy spectrum of the harmonic oscillator.

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RNS Superstring Theory with Deformed Energy–Momentum Relations in the Presence of a Dust Field

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We investigate a modified closed bosonic string theory incorporating deformed dispersion relations in the presence of a dust field, which is modeled as a real scalar field on the string worldsheet. Employing the Hamiltonian formalism, we systematically address the associated constraints. One of these constraints is linear in the dust field momentum, allowing us to impose a dust time gauge that leads to a non-vanishing physical Hamiltonian. In contrast, the spatial diffeomorphism constraint remains identically zero. We show that the commutation relations between the string modes are affected by the presence of the deformed dispersion relations. Upon quantization, the theory is found to be consistent in spacetime dimensions $D < 26$, and the resulting spectrum depends on an additional parameter that can be tuned to eliminate tachyonic states.

Keywords:
Quantume gravity, dust gauge, despertion relations, contraintes.

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Thermodynamic properties and non-relativistic Treatment of Spinless Particles Subject to time dependent Yukawa potential via the Nikiforov- Uvarov-Functional Analysis method

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The time dependent Schrodinger equation for the Yukawa potential is studied. The potential is not studied in literatures. It has been used in non-relativistic quantum mechanics to study the interaction between non-relativistic particles. To obtain the energies spectrum and the wave function we use a new method for solving a second order differential equation of the hypergeometric type called Nikiforov-Uvarov Functional Analysis (NUAF) method and the method of variables sepration.

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Effects of APD Photodetector Thermal Noise in the Optical Networks

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We study the effects of using avalanche photo diode (APD) Photo detector Thermal Noise in the Long-distance optical networks with 32 number of users and compare the efficiency of the bit-error-rate (BER) and quality (Q)-Factor. The research is conducted using (APD) receivers of different wave lengths.Interpretation and description of the Optic system's simulation results through the optical high debit communication system in order to provide new perspectives for the future transmission.

Background/Introduction:

In this work we intend to analyze the performance of using avalanche photo diode (APD) photodetector thermal noise in the Long-distance optical networks with 32 number of users using different fiber lengths, CW laser powers, data rates and number of users, by calculating BER and quality Q-factor.

Objective: The aim of this study is to examine the noise of photo detection coursed in APD photodiodes used as detectors in the transmission chain .Taking into account that the transmission quality achieved with Q>6.to guarantee a BER less than 10-9

Keywords:
APD - Thermal Noise – Q Factor – BER.

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Standard Model

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Azimuthal distribution of the γ emitted in association with the Z boson: a good indicator for testing the accuracy of the standard model?

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The azimuthal distribution constitutes a central analytical tool in particle physics due to its precision in testing standard model predictions. This work presents a phenomenological study of the emission of a photon in association with a Z boson in proton-proton collisions, using modified Feynman rules up to first order in the noncommutative parameter Θ,we employ computational tools ,such as the FeynCalc package in Mathematica, alongside analytical methods as MadGraph and MadAnalysis to extract the cross-section and azimuthal distributions, which allow for the exploration of potential deviations from the standard model with high accuracy.

Keywords:
Standard model, Azimuthal distribution, NCSM.

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Study of CP Violation in Λb baryon decays in BLSSM with Inverse seesaw

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Recently, the LHCb collaboration observed CP violation in the beauty-lambda baryon $\Lambda_b \to J/\Psi\, pK^- \, (\pi^-)$ decays. The direct CP asymmetry in Λb decays is an intriguing hint for new physics beyond the Standard Model. We investigate the CP violation effect on $\Lambda_b \to \Lambda_c\ \tau\nu$ decays in BLSSM with Inverse seesaw.

Background/Introduction:

Recently, LHCb collaboration reported that the ratio $R(\Lambda_c)_{exp} = 0.242 \pm 0.076$ which deviates by 1.1σ from the standard model prediction $R(\Lambda_c)_{SM} = 0.324 \pm 0.004$. In this talk we show that the CP Violating complex parametrs in B—L extension of the Supersymmetric Standard Model with inverse Seesaw mechanism might explain this deviation.

Objective:

The main goal of this work is to explain the above deviation.

Methods:

We study the Λb baryon decay through the observable $R(\Lambda_c)$ which is defined as the ratio of decay rates of the transition $b \to c\, l\, \nu\ (l = e, \mu, \tau)$. The BLSSM-IS contributions to the ratios $R(\Lambda_c)$ primarily arise from penguin box, mediated by the exchange of charginos and neutralinos together with righthanded sneutrinos. In our numerical analysis we used some hep tools.

Conclusion/Implications:

Although the current experimental uncertainties in $R(\Lambda c)$ are still large. Due to the *presence of CP violation,* our results highlight a potential correlation with the mesonic ratios that can be tested more stringently in future measurements.

Keywords:

Supersymmetry, Λb baryon decay, LFU

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Flavor-Changing Neutral Currents in the Flipped 341 Model

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Background/Introduction:
The flipped 341 model, based on the gauge symmetry $SU(3)_C \times SU(4)_L \times U(1)_X$, provides an appealing framework for exploring physics beyond the Standard Model, particularly in the flavor sector. The model predicts new neutral gauge bosons and scalar fields that can induce flavor-changing neutral currents (FCNCs) at tree level, offering a rich structure to study flavor violation in leptonic processes.

Objective:
This work aims to analyze the origin and behavior of FCNCs in the flipped 341 model and to determine their possible low-energy signatures, focusing on the leptonic sector.

Methods:
We identify the interactions responsible for FCNCs and derive the relevant couplings in both the extended gauge and scalar sectors. Several leptonic and semi-leptonic decay channels are investigated, including the three-body decays $\tau \to \mu ee$ and $\tau \to e\mu\mu$, the semi-leptonic processes $\tau \to \mu$ and $\tau \to e$, as well as μ–e conversion in nuclei. Analytical expressions for the corresponding decay amplitudes and branching ratios are obtained in terms of the model parameters.

Results:
The nonuniversal couplings of lepton families to the new neutral gauge bosons Z' and Z'' give rise to tree-level FCNCs with measurable effects. Using current experimental bounds on the above processes, we derive constraints on the masses of the new gauge bosons and the strength of the flavor-changing parameters.

Conclusion/Implications:
Our results show that the flipped 341 model can produce observable FCNC effects in forthcoming flavor experiments, particularly in precision searches involving τ and μ decays. These findings highlight the model's potential to provide complementary signatures of new physics beyond the Standard Model.

Keywords: Flipped 341 model, flavor-changing neutral currents, leptonic decays, μ–e conversion, new physics

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Cosmology

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Thermodynamics of the Schwarzschild Black Hole in Noncommutative Gauge Gravity

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In this study, we used the non-commutative (NC) gauge theory of gravity to analyze the thermodynamic properties of a deformed Schwarzschild black hole (SBH). We obtain the NC Hawking temperature correction. We show that the noncommutativity removes the divergence behavior of temperature and these corrections reveal an estimation of the NC parameter Θ which is found at the Planck scale order, Θ ∼ lplanck. Then, the description of the heat capacity of the deformed black hole shows the effect of the NC geometry on the thermodynamic stability and the phase transitions.

Objective:

The goal is to describe gravity through a Schwarzschild solution using the gauge theory in non-commutative space time, and to study its thermodynamic properties. Clearly state the aim or research question your study attempts to answer.

Results:

Our results demonstrate that the non-commutativity removes the divergent behavior of the temperature. We also find that the non-commutativity of space time is significant at the Planck scale.

Conclusion/Implications:

In this work, we study the modified thermodynamics of black holes in a NC theory of gravity. Our corrections distribute the singularity at r = 0 over a twodimensional sphere with radius r = 2 m, and the new event horizon is increased by the NC correction, rNC h > rh. We show that the non-commutativity of space time modifies the thermodynamic properties of the black hole, such as its temperature, entropy, and heat capacity. Our results demonstrate that the noncommutativity removes the divergent behavior of the temperature. We also find that the non-commutativity of space time is significant at the Planck scale. Explain the significance of your results. What do they mean in a broader context? How do they contribute to the field or solve the problem introduced?

Keywords:

Schwarzschild black hole, non-commutative gauge theory, the thermodynamic properties

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Spontaneous Scalarization of Neutron Stars in Scalar Torsion Theories

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Spontaneous scalarization of neutron stars (NS) is a phase transition mechanism that triggered at linear level by a tachyonic instability, which arises from a negative effective mass of the scalar field. This study explores the possibility of such scalarization occurring within the context of teleparallel scalar-tensor theories of gravity, namely scalar torsion gravity. In our work, we promote the TEGR action to include scalar fields, which interact minimally to gravity and consider a linear form of the coupling scalar function. The 39btained39 equations for slowly rotating isotropic NS are derived for different equations of state, then integrated numerically for both interior and exterior regions using the39btaine conditions near the center, and the asymptotic boundary conditions at large distances for the metric functions and the scalar field. Our findings reveals the existence of scalarized branch of solutions for both positive and negative values of the coupling parameter beside the standard GR branch. The 39btained results allow for probing the strong field regime, and explore alternative formulations of gravity consistent with observational data.

Keywords:

neutron stars, spontaneous scalarization, teleparallel gravity, scalar torsion.

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Noncommutative Black Cosmic String

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Using the W.K.B. approximation and the Hamilton-Jacobi method, noncommutative corrections to the Hawking temperature of the quantum tunneling radiation of Dirac fermions through the horizon of a black noncommutative Kerr-Newman cosmic string were studied.

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The contribution of Inverse Compton scattering to GRB afterglows

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The Gamma-Ray Bursts are among the brightest and most powerful events in the universe. The interaction of the burst source with the surrounding medium is referred to as afterglow. In this work, we use synchrotron emission as the basis for modeling the light curve. However, the influence of the Inverse Compton scattering becomes significant at high energies.

Background/Introduction:
The inverse Compton process occurs when a photon is scattered by an ultra-relativistic charged particle. At high energies, this process has an influence on GRB afterglows.

Objective:
This study will examine the effect of Inverse Compton scattering on the GRB Afterglows, when a photon collides with an ultra-relativistic charged particle, gaining additional energy.

Results:
Inverse Compton affects the Afterglow of the gamma-ray burst at high energies.

Conclusion/Implications:
The Inverse Compton effect is fundamental to realistic GRB models and helps understanding the physical conditions in the emission region.

Keywords:
Inverse Compton scattering, GRB afterglows, synchrotron emission

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First Principle Derivation of Stochastic Ricci Flow: Tensorial Geometrization and Resolution of the Cosmological Constant

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This work atempt to adresse one of the central challenges of modern theoretical physics — the derivation of spacetime dynamics from quantum principles without assuming the prior existence of time or metric. Building on the framework of Tensor Field Theories (TFT) and the concept of relational time, it aims to bridge discrete quantum structures with continuous geometry.

Objective:

The objective is to derive, from first principles, the Stochastic Ricci Flow (SRF) equation as the emergent dynamical law of spacetime, providing a structural solution to the Problem of Time and a natural resolution of the Cosmological Constant (Λ) problem.

Methods:

The study begins with renormalizable TFTs defined in a timeless global state ($\hat{H}|\Psi\rangle = 0$). The Gurau degree (ω) is introduced as a topological measure of discrete complexity, acting as a functional minimized through a gradient flow. In the continuous limit ($N \to \infty$), this flow converges toward the Ricci functional $\int R\sqrt{g}\, dx$, yielding a continuous geometric evolution. By including stochastic fluctuations ξ_{ij} proportional to $\hbar$, the resulting equation generalizes Hamilton's Ricci flow into its stochastic form.

Results:

The derived Stochastic Ricci Flow equation is:

$$\partial_t g_{ij} = -2R_{ij} + \xi_{ij}(x,t) + \nabla_i \nabla^j \varphi + \Lambda g_{ij}.$$

Each term encodes a specific physical origin:

(i) curvature smoothing by ω-minimization,

(ii) quantum fluctuations represented by noise ξ_{ij}, and

(iii) an emergent scalar mode φ from tensor condensation.

The cosmological constant Λ emerges naturally as a topological residue of the combinatorial structure rather than as a fundamental constant.

Conclusion/Implications:

This unified framework shows that General Relativity can be viewed as the fixed point of a quantum-combinatorial regularization process. The theory predicts measurable stochastic corrections to spacetime curvature and a first-principle expression for Λ. It thus offers a consistent geometrization of quantum gravity linking discrete tensorial dynamics to continuous relativistic geometry.

Keywords:

Quantum Gravity, Tensor Field Theories, Stochastic Ricci Flow, Cosmological Constant, Geometrization

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Theoretical Chemistry

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The Intelligent Research Assistant: Automating Molecular Geometry Comparison and Data Extraction with AI"

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The increasing complexity of computational chemistry workflows, employing software such as Gaussian, ORCA, and MOE, generates vast and heterogeneous data. Manually parsing output files to extract molecular geometries, energies, and spectroscopic properties is a significant bottleneck, prone to error and impractical for high-throughput studies. This lecture will explore the transformative role of artificial intelligence (AI) in automating and enhancing these critical postprocessing tasks. We will demonstrate how machine learning models, particularly natural language processing (NLP) and computer vision, are being developed to intelligently parse complex result files[1-3]. These AI assistants can automatically identify and extract optimized molecular geometries, vibrational frequencies, and electronic transition energies, converting unstructured text into structured, queryable databases. A key application is the quantitative comparison of molecular geometries. AIdriven tools can systematically analyze bond lengths, angles, and dihedrals across a dataset of calculations, identifying conformational trends and anomalies that might be missed by manual inspection. Furthermore, we will present frameworks that leverage AI to correlate extracted geometric parameters with computed energetic and electronic properties, facilitating the discovery of structure-property relationships. This integration streamlines validation, accelerates data analysis, and enables the mining of existing computational datasets for new insights. By acting as an intelligent intermediary between the raw output of specialized software and the researcher, AI is poised to significantly accelerate the discovery cycle in theoretical and computational materials chemistry.

Keywords:
Artificial Intelligence, Computational Chemistry, Data Mining, Molecular Geometry, High-Throughput Screening.

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Étude des propriétés magnétiques de complexes diuranium U(IV)-U(IV) par l'application de la théorie DFT relativiste couplée à l'approche de symétrie brisée (BS).

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Les matériaux moléculaires magnétiques, notamment les complexes d'actinides, suscitent un vif intérêt en recherche. Ces systèmes, où des centres métalliques sont reliés par des ligands pontants, présentent des échanges magnétiques ferromagnétiques ou antiferromagnétiques. Le concept de super-échange d'O. Kahn [1], a été fondamental pour développer ces matériaux, conduisant aux Aimants Moléculaires Uniques (SMM) [2].

L'étude théorique de leur magnétisme est complexe, mais les avancées en calcul et en méthodes quantiques comme la Théorie de la Fonctionnelle de la Densité (DFT) et son approche à symétrie brisée (DFT-BS) ont permis de modéliser ces propriétés [3]. Le comportement magnétique est fortement influencé par la nature du ligand pontant et l'environnement structural des métaux.

Nos recherches se concentrent sur l'étude théorique de complexes diuranium U(IV) pontés par des ligands éthynediyl-bispyrazine et imino-amido quinoïdes. En utilisant une méthode relativiste (DFT/ZORA/TZP/B3LYP) via le code AMS, nous démontrons que l'approche par symétrie brisée reproduit fidèlement leur comportement magnétique. Elle confirme une interaction antiferromagnétique entre les centres U(IV), en parfait accord avec les données expérimentales. Cette étude met en lumière le rôle crucial des orbitales 5f de l'uranium dans les interactions métal-ligand et la communication électronique U($5f^2$)-L-U($5f^2$), qui est essentielle au mécanisme d'échange magnétique.

Key words:

Magnétique moléculaires, constante d'échange magnétique, la théorie de densité fonctionnelle, broken symmetry (BS).

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From VQE to SQD: Modern Quantum Algorithms for The Electronic Structure Problem

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Accurately determining molecular ground-state energies remains a central challenge for computational chemistry. Classical exact methods such as Full Configuration Interaction scale exponentially with system size, while quantum approaches like the Variational Quantum Eigensolver (VQE) face fundamental limitations, including barren plateaus and a rapid increase in measurement overhead. This work investigates two recently introduced sampling-based algorithms, Quantum-Selected Configuration Interaction (QSCI) and Sample-Based Quantum Diagonalization (SQD), as promising near-term alternatives to VQE. The objective is to analytically characterize their sampling behavior and identify the dominant factors that limit their scalability. Both methods employ a quantum processor solely to sample Slater determinants, while the Hamiltonian diagonalization is performed classically, thereby avoiding the need for variational optimization. The central contribution of this study is the derivation of an analytical model for the determinant-discovery process by establishing a direct analogy with the classical coupon collector problem. This mapping leads to the first exact expression and a scalable lower-bound estimator for the expected number of projective measurements required to recover all determinants contributing to the ground state. The theoretical predictions are validated through a comprehensive set of numerical and experimental tests, including ideal state-vector simulations, hardware-calibrated noisy simulations, and real-device runs on IBM's 127-qubit Brisbane processor. The results confirm the theoretical scaling and highlight the sampling bottleneck as the dominant cost in QSCI and SQD. This work provides a quantitative framework for understanding sampling efficiency in measurement-based quantum diagonalization algorithms and clarifies the trade-off between sampling cost and scalability, offering valuable insights for designing more measurement-efficient post-VQE quantum algorithms in chemistry.

Keywords: Quantum algorithms, Sampling-based Quantum diagonalization, Quantum chemistry, Quantum-Selected Configuration Interaction, Variational Quantum Eigensolver.

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AI and Others

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An Artificial Intelligence-Based Approach for Enhancing the Sustainability and Productivity of Agricultural Greenhouses

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This paper provides a comprehensive overview of an integrated smart agricultural platform designed to monitor, control, and optimize the greenhouse environment. The platform utilizes sensors to collect real-time data, applies machine learning algorithms to predict environmental conditions, and provides a control system for automating agricultural operations. The project aims to increase resource efficiency, improve crop health, and boost productivity through data-driven precision agriculture. The platform is constructed using modern software architecture, including a Python-based backend and an interactive React frontend. This report details the system architecture, the adopted methodology, the mathematical foundation of the models, preliminary results, and future plans for platform development, with a focus on the importance of developing hybrid models and collecting high-quality data to ensure model reliability and generalizability.

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Poster Sessions

Nuclear Physics Applications

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Development of Monte Carlo simulation correction models to improve the detection limits of Instrumental Neutron Activation Analysis technique: Determination of lanthanide elements in Algerian phosphates

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In this work, the instrumental neutron activation analysis technique was exploited for the precise determination of the concentrations of lanthanides present in phosphate samples collected from the Jebel El Onk phosphate deposit, in eastern Algeria, which contains ignificant mineral resources, uranium, and thorium, with reserves estimated at more than 2 billion tones in this region. Instrumental Neutron Activation Analysis (INAA) is a very ffective method for analyzing low-level elements in environmental samples, notably phosphates. However, the presence of REEs and phosphorus in the phosphate sample affects the detection limit of the technique. The irradiation of phosphate samples under a neutron flux in a nuclear reactor is affected by the local disruption of the neutron flux produced mainly by the sample. The presence of phosphorus in the phosphate matrix leads to the production of 32P under thermal flow irradiation. This radioelement presents a Bremssatrlhung (background) spectrum which influences the gamma spectrum of the rare earth elements in the sample. Thus, it affects the detection limits of the method. The irradiation and measurement parameters must be corrected to ensure highly accurate analysis. An analysis methodology has been developed. Based on Monte Carlo simulations and experimental easurements for the calibration of the efficiency of the HPGe detector, the optimization of the filter thickness to reduce Bremsstrahlung noise, and the estimation of the neutron self-absorption factor, thermal, and epithermal. The methodology developed improved the detection limits, allowing high precision for determining the contents of REEs such as La, Nd, Eu, Sm, Ce, Tb, Yb, and Hf in phosphate samples from the Bled El deposits Hadba. The results obtained can serve as a valuable database for the future exploitation of these resources.

Keywords: Instrumental Neutron Activation Analysis, Neutron self-shielding, Monte Carlo Simulation, Reduction of the beta spectrum, Detection Limit, Lanthanide concentrations, Phosphate.

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Experimental Study of Intrinsic Background and Response function of Cerium Doped Lanthanum Bromide Scintillator Detector

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In nuclear physics, the quantification of the radionuclides, even in laboratory or in situ measurement, required a wide range of spectrometers where the linearity on energy eposit, high detection efficiency, low energy resolution, fast timing response, etc, could be found in he used spectrometer.

Background/Introduction:

Recently, the lanthanum-based detectors were presented as commercial spectrometers applied in nuclear physics, radiation monitoring, dosimetry applications, etc.

Objective:

In this study, we aim to evaluate the response function of a 1.5"×1.5" LaBr3(Ce) scintillator detector by experimental data and the unfolding process.

Methods: A series of measurements in time units was adopted to evaluate the evaluation of the intrinsic background level. Experimentally, several gamma radiation sources were used to determine the energy resolution and efficiency curves.

Results:

The results show that: (1) a non-ignored level of intrinsic radiation is registered; (2) excellent low values of energy resolution close to HP(Ge) detector; (3) a good linearity on incident and deposit energy.

Conclusion/Implications: The results are encouraging for the use of these kinds of detectors after internal background subtraction and the deconvolution process

Keywords:

^{138}La, LaBr3(Ce) detector, GEB, spectrometry, Fredholm integral.

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Nuclear Data Evaluation for (p,n) Reactions Using Semi-Empirical Modeling

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Background/Introduction:

The (p,n) reactions play a crucial role in nuclear physics and technological applications, particularly in radioisotope production and neutron activation analysis. Updating evaluated data for these reactions at energies of 7.5 and 12.4 MeV is essential for improving calculation accuracy in these application domains.

Objective:

This study aims to develop a new semi-empirical formula for accurately calculating cross-sections of (p,n) reactions at energies of 7.5 and 12.4 MeV, with the goal of improving available nuclear data.

Methods:

The adopted approach combines several existing nuclear models including the statistical model, pre-equilibrium model, and direct reaction mechanisms. These models were used to develop an optimized semi-empirical formulation that accounts for specific characteristics of (p,n) reactions at the considered energies.

Results:

The calculations generated graphs representing experimental, calculated, and evaluated cross-section values as a function of proton energy. The study enabled the integration of new isotopes and obtained good values for statistical parameters, showing satisfactory agreement between theoretical and experimental data.

Conclusion/Implications:

This new semi-empirical formula contributes significantly to updating existing nuclear data libraries such as ENDF. The integration of new isotopes and optimization of statistical parameters improve calculation accuracy for applications in applied nuclear physics. Future work will extend this formula to higher energies and explore integration into Monte Carlo and Talys simulation codes for broader applications.

Keywords: (p,n) reaction, cross-section, semi-empirical formula, statistical model, pre-equilibrium

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Synthesis, Charactérization and Nuclear Application of Mesoporous Silica: MCM-48

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Mesoporous materials have emerged as promising adsorbents for the treatment of radioactive waste due to their high surface area, tunable pore size, and excellent chemical stability. These properties enable the efficient capture and immobilization of hazardous radionuclides from contaminated effluents. Mesoporous silica MCM48 was synthesized via a hydrothermal method using tetraethyl orthosilicate (TEOS) as the silica source and cetyltrimethylammonium bromide (CTAB) as the surfactant under basic conditions. The structural and morphological characteristics of the resulting nanopowders were investigated through a complementary set of techniques, including X-ray diffraction (XRD), nitrogen adsorption–desorption (BET), and scanning electron microscopy (SEM), to elucidate their physicochemical and morphological properties. Subsequently,
the samples were subjected to gamma irradiation at doses ranging from 0 to 1000 Gy to evaluate its effect on the removal efficiency of heavy metals, specifically Cu (II), Ni (II), and Co (II), which are relevant to nuclear facility decontamination. The synthesized materials exhibited high specific surface areas, uniform pore size distributions, significant pore volumes, and excellent thermal stability, underscoring their potential as versatile candidates for applications in catalysis, adsorption, and related fields.

Key words:
Mesopourous materials, MCM-48, Gamma irradiation, XRD, BET, SEM.

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Theoretical study of the ionization of atoms by electron impact

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Background/Introduction:

Our study focuses on calculating the triple differential cross sections (TDCS) of ionization for the two atoms 'Helium and Neon' to understand the changes in the internal structure of these atoms, as well as the collision mechanisms.

Objective:

The objective is to calculate the triple differential cross sections (TDCS) as a function of the ejection angle for different values of incident energy (Ei) and ejection energy (Ee).

Methods:

In this study, we develop the calculation of triple differential cross sections in the first Born approximation (FBA) using Clementi's wave function [1] to describe the bound state of the atom. The frozen core approximation and the single-particle picture model were used to reduce the N-electron problem to one-electron problem.

Results:

Our results are perfectly consistent with the experimental results of [2-3] in the high-energy range.

Conclusion/Implications:

Our results are in good agreement only in the high-energy range. To improve them in the low-energy range, we suggest using Born's second approximation. We conclude that the choice of theoretical models and wave functions describing the bound state of the atomic target plays a very important role in describing the ionization process.

Keywords:

Ionization, Cross-Section, Coulomb wave.

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Band Structures Study in Even-A Xenon isotopes WithinCranking Nilsson Strutinsky Model

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To investigate the shape evolution of xenon isotopes in the mass region A = 112–132, the *Cranking Nilsson-Strutinsky* (CNS) model is employed. Energy level calculations are performed and compared with experimental data. Additionally, potential energy surfaces as functions of the deformation parameters ($\varepsilon 2$, γ) are generated to illustrate the shape evolution of these nuclei near the Z = 50 proton shell.

Keywords:
Xenon isotopes, CNS Model, Energy Levels, Potential Energy Surfaces

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Optimizing Prostate Radiotherapy: Impact of Delivery Technique (Sequential IMRT vs SIB) and Beam Energy

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Background/Introduction:
Intensity-Modulated Radiation Therapy (IMRT) has become the main treatment mode in prostate cancer radiotherapy, offering highly conformal dose distributions and improved sparing of surrounding organs at risk (OARs). Two main ballistics are commonly used: the sequential and the Simultaneous Integrated Boost (SIB) IMRT techniques. In parallel, advances in linear accelerator technology have introduced flattening filter-free (FFF) photon beams, which provide higher dose rates up to 1400 UM/Min and potentially reduced treatment times compared with conventional 18 MV beams. The clinical and dosimetric implications of combining these different delivery techniques and beam energies remain an area of active investigation.

Objective: This study aims to compare the dosimetric performance and efficiency of sequential IMRT versus SIB techniques in prostate cancer treatment, Moreover, to evaluate the impact of different photon beam energies 18 MV and 6 FFF on target coverage, OAR sparing, and treatment delivery time.

Methods: This study was performed by generating treatment plans for a cohort of prostate cancer patients using both sequential IMRT and SIB techniques. Thus, for SIB technique, each plan was created with 6 FFF and 18 MV photon beams on a Truebeam accelerator in radiotherapy department of Constantine University Hospital Center, maintaining consistent planning objectives and dose constraints based on institutional and international guidelines. Dosimetric parameters, including PTV coverage, conformity, homogeneity, and OAR doses (rectum, bladder, femoral heads), were analyzed. Treatment efficiency was assessed through monitor units (MU) and beam-on time.

Results: Preliminary study showed that SIB plans achieved comparable or superior PTV coverage with improved conformity and reduced overall treatment time compared to sequential IMRT. Although, OAR doses were much lower in sequential plans than in the SIB ones. The use of 6 FFF beams significantly decreased beam-on time without compromising dose homogeneity. However, 18 MV plans exhibited slightly improved deep tissue dose uniformity at the cost of higher neutron contamination potential and longer treatment duration.

Conclusion/Implications: In prostate cancer radiotherapy, SIB with 6 FFF photon beams provides an optimal balance between dosimetric quality and treatment efficiency. These results support the use of advanced delivery techniques and modern beam energies to enhance precision, reduce treatment time, and improve patient comfort.

Keywords: Prostate, IMRT, SIB, sequential, flattening filter-free, beam energy

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Magneto-Inertial Fusion in Nuclear Physics: Comparative Theoretical Analysis and Energy Implications

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Background/Introduction:
Magneto-Inertial Fusion (MIF) represents a promising hybrid approach in nuclear physics that combines the advantages of magnetic and inertial confinement schemes to achieve controlled thermonuclear fusion. Despite extensive theoretical and experimental studies, discrepancies remain between different models in describing plasma compression, confinement efficiency, and the mechanisms governing plasma stability.

Objective:
This study aims to perform a comparative theoretical analysis of major MIF models to clarify how magnetic field strength, plasma density, and kinetic instabilities influence confinement performance and fusion energy gain.

Methods: The analysis is based on a synthesis of fundamental theoretical frameworks, including the works of Lindemuth (1983), Slutz (2010), Hsu (2005), and Freidberg (2014). These models are compared through their governing equations for energy balance, magnetic compression, and instability growth, with particular attention to the Weibel and Rayleigh–Taylor modes that can disrupt implosion symmetry.

Results: The comparative study shows that MIF configurations incorporating axial magnetic pre-compression improve confinement time and energy efficiency relative to purely inertial models. However, magneto-hydrodynamic (MHD) instabilities remain a critical limiting factor affecting plasma compression symmetry and overall fusion yield.

Conclusion/Implications: This analysis highlights the importance of integrating magnetic and inertial confinement mechanisms within nuclear fusion research. Understanding and controlling plasma instabilities are essential for improving plasma stability and advancing the feasibility of magneto-inertial fusion as a sustainable and clean energy source.

Keywords: Magneto-Inertial Fusion, Nuclear Physics, Plasma Instabilities, Magnetic Compression, Energy Applications.

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Assessment of fast neutron flux by aluminum activation technique

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This study primarily focuses on the measurement of nuclear reaction cross sections. Accurate determination of the incident neutron flux to which the samples are exposed is therefore essential. The measurements were performed using a neutron generator of the "SAMES J-25" type, which is a low-energy accelerator. Fast neutrons were produced through the ^{3}H(d, n)^{4}He nuclear reaction, generating neutron energies in the range of 13.4 to 14.75 MeV, depending on the energy of the incident deuterons and their emission angle. The Neutron Activation Analysis (NAA) technique was employed using high-purity aluminum foils (99.9999%). The ^{27}Al(n, α)^{24}Na reaction was used as a flux monitor because of its well-known cross section and favorable radioactive decay parameters for neutron activation measurements. The irradiation time was optimized to avoid saturation while ensuring good counting statistics. The irradiated aluminum foils were successively placed in front of a high-purity germanium (HPGe) detector, positioned identically to the ^{152}Eu calibration source used for detector efficiency determination. The resulting gamma-ray spectra were analyzed using the Genie-2000 software. The obtained results confirm the reliability of the ^{27}Al(n, α)^{24}Na reaction for fast neutron flux measurement and dosimetry applications.

Keywords:
NAA, Fast neutron flux, HPGe gamma spectrometry.

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Empirical calculation of jump ratios rk for selective elements

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The K-shell absorption jump ratio (r_K) is a key atomic parameter for X-ray imaging, detector calibration, and radiation modeling. This study develops new empirical r_K values for elements with Z = 32–39 using second-order polynomial interpolation of experimental data. The derived ratios show strong agreement with existing experimental and theoretical results. This confirms the accuracy of the proposed model and its utility in providing reliable parameters for understanding electronic transitions and improving X-ray based applications.

Background:

Background: The K-shell absorption jump ratio is a fundamental atomic parameter that dictates how sharply a material's X-ray attenuation changes at its characteristic K-edge energy. This sharpness directly translates to performance in advanced imaging techniques (spectral CT, K-edge imaging), detector design and efficiency, contrast agent efficacy, and accurate radiation dose modelling, particularly for the specified elements used in these technologies. Precise knowledge of these ratios is essential for system design, calibration, image reconstruction, and quantitative analysis. The theoretical, experimental, and analytical methods for calculating jump ratios for various elements are significant due to their numerous applications. Based on available experimental values of r_K, we propose new empirical values for the K shell absorption jump ratios. Our results align well with theoretical values, showing good agreement.

Objectives:

This study aims to:

Develop and propose new empirical values for the K-shell X-ray absorption jump ratios (r_K) for elements with atomic numbers Z=32 (Ge), 33 (As), 34 (Se), 35 (Br), 36 (Kr), and 39 (Y)

Validate these newly derived empirical values by comparing them with existing experimental and theoretical data.

Demonstrate the applicability and reliability of the proposed empirical approach for accurately characterizing K-shell absorption jump ratios.

Methods:

This study introduces novel parameters for determining K shell absorption jump factors and jump ratios for selective elements with atomic numbers in the range $32 \leq Z \leq 39$. The empirical values of r_K were derived using the mathematical approach of polynomial interpolation 2 order, based on experimental data published between 1986 and 2016.

Results:

polynomial interpolation 2 order was employed to calculate the k shell absorption jump ratios for elements with atomic numbers ranging from 32 to 39. These calculated values were then compared with experimental and theoretical values. The results obtained generally align with both experimental and theoretical values across the entire range of elements ($32 \leq Z \leq 39$). Results demonstrate strong concordance with experimental findings, with deviations confined to a narrow range of 0% to 4%. This close alignment underscores the model's robustness and reliability.

Conclusion:

Empirical methods accurately characterize atomic jump parameters, consistent with previous research. This validates the method's predictive power and enhances understanding of electronic transitions in atoms.

Keywords:

X-ray; K shell absorption jump ratio; analytical function; empirical calculation.

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Etude of the electric properties of polymers of polyethylene naphtalate (PEN) in films using the final current method

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Polymers are frequently used as electrical insulation materials and can be found in capacitors, space equipment, and nuclear power plants. In these contexts, various materials are subjected to various mechanical, electrical, and thermal stresses. These elements are responsible for modifying the physical, chemical, and mechanical characteristics of the material, which manifests itself in processes of chain breakage, cross-linking, and oxidation. In this study, we analyzed electrical behavior using the final current method to evaluate the deterioration of the polymer under the influence of temperature.

Background/Introduction:

In this study, we examine the electrical properties of PEN under the influence of temperature using the final current method to evaluate polymer degradation.

ObjectiveMy study consists of verifying whether exposing polymers to thermal stress will increase the degree of polymer degradation.

Methods: In this work, measurements are taken on a 25 μm thick polyethylene naphtalate (PEN) polymer film metallized on both sides with a 30 nm thick layer of gold to ensure good electrical contact during electrical current measurements.

Results:

The temperature-dependent change of the non-isothermal discharge current can result in one or more picture shapes. This effectively illustrates the existence of a non-nuclear charge in the echantillon that releases itself following a thermal energy gain during heating.

Conclusion/Implications:

When the temperature of the non-isothermal discharge temperature increased, the finaux current measurements in the PEN films showed an increase in the value of the non-isothermal discharge currents, or CDF, traced in relation to temperature.

Keywords: PEN, final current, piege.

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Transmutation Efficiency of Iodine-129 Long Lived Fission product

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Transmutation of nuclear waste after its separation is an effective way to dispose of it. Transmutation principle is based on the transformation of radioactive element by a nuclear reaction to another less radioactively element or stable.

The objective of this work is to study the destruction of Iodine-129 as an example of application in three high flux nuclear reactors Petten (Netherlands), BR2 (Belgium) and SM3 (Russia).

Transmutation efficiency is obtained from the ChainSolver and ChainFinder 2.34 calculation codes. The numerical results are simulated for an irradiation time of 300 effective full power days (EFPD). The results are then compared to choose the best reactor to destroy iodine-129.

The SM3 high flux reactor seems to be the best High Flux Reactor that offers the highest value of iodine-129 Transmutation Support Ratio (TSR) and Average Transmutation Acceleration (A)

To accelerate the transmutation of iodine according to irradiation time in HFRs, the thermal and epithermal neutron fluxes must be as high as possible, this based on the neutron-section of Iodine-129 in the epithermal and fast region.

Keywords:
Iodine, Transmutation, ChainSolver, ChainFinder, HFR

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Simulation of the fluorescence signal detected by a space telescope for extreme energy cosmic ray observation

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The experimental technique of fluorescence light measurement is used for indirect observation of cosmic ray particles at very high energies. Extensive air showers (EAS) initiated by extreme energy cosmic rays (EECRs), up to 100 EeV and entering the Earth's atmosphere, are simulated with the CORSIKA package. Influence of different simulation parameters on the EAS characteristics is studied, especially on longitudinal distribution of charged particles, depth of shower maximum and energy released to the air. By taking the atmospheric scattering of light into account, the number of fluorescence photons, with wavelengths between 300-430 nm, and their arrival time distribution to an ideal space telescope are calculated.

Background/Introduction: Ultra High Energy Cosmic Rays (UHECR) are the most energetic particles observed in nature with (detected) energies up to 3-5.1020 eV. The experimental observations of UHECR are performed nowadays by the Auger observatory in Argentina and Telescope Array (TA) observatory in the USA. JEM-EUSO is a new type of observatory, embarked on the ISS, that uses the whole Earth as a detector. The observation of these particles leads to many interesting questions mainly on their nature and origin.

Objective: In this work, we have performed an calculation of the amount of fluorescence photons arriving at the detector pupil of JEM-EUSO.

Methods: we use the simulation by Corsika, model QGSJETII-04 for high energy and GHEISHA for a low energy , we calculated by it the energy deposit.

We have studied the Fluorescence yield for the US standard atmosphere, between 300 and 430 nm in air, we use the energy deposit rate and to take into account the attenuation of photon in the air (Rayleigh scattering).

Results:

Our calculation for a 500 proton and 500 iron of $\boldsymbol{E}$=**1020** eV and 60° has given 7055 ± 96.3414 and 7406 ± 48.6677 fluorescence photons arriving at the detector respectively

Conclusion/Implications: Our calculation is in a good agreement with a more precise calculation done by M. Bertaina using the EUSO Simulation and Analysis Framework (ESAF) that has given 7 131 fluorescence photons arriving.

Keywords: Cosmic rays, JEM-EUSO, CORSIKA sumilation, Extensive air showers, Fluorescence yield.

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Clinical implantation of flattening filter free (FFF) photon beams in radiotherapy

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The flattening filter-free (FFF) photon beams are often incorporated into the clinical practice of modern radiotherapy. It is necessary to discuss the use of this beam for treatment delivery separately for each technique. The purpose of this study is to evaluate the dosimetric quality when planning treatments with FFF beams as compared to standard flattened beams (FF).

Treatment plans were created for different patients and cancer sites, with or without the use of a flattening filter for photon beams of 6 and 10 MV energies from a "True Beam" linear accelerator, all plans were generated in the 'Eclipse' treatment planning system (TPS) and calculated using the analytical anisotropic algorithm (AAA). The quality of FFF beam plans was estimated by conducting a dosimetric comparison between plans with and without a flattening filter. Various parameters were used to analyze the evaluation of the planning target volume (PTV) and organs at risk (OAR).

The mean dose and coverage of the PTV were not significantly different between FFF and FF plans according to the dose-volume histogram and isodose curve analysis. However, the OAR uncovered a minor difference. Although the two beam modes have similar MUs, FFF beams have a significantly shorter beam-on time due to their high dose rate. The results obtained are in good agreement with those reported in the literature for other planning systems and techniques.

The FFF photon beam obtained dosimetric quality similar to that of the standard flat beam, which enables the development of improved radiation treatments with shorter delivery times and lower doses to normal organs.

Keywords: Flattening Filter Free (FFF), clinical implentation, High dose rate, Dosimetric quality

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Quantum Information

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Entanglement Properties of Mesoscopic Trapped Systems under Kratzer-Type Interactions

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This work presents a theoretical investigation of multipartite quantum entanglement in mesoscopic systems confined in a harmonic oscillator trap and interacting via a Kratzer potential. The Kratzer potential provides a realistic model for interparticle interactions, combining attractive and repulsive components. By constructing and analyzing the total Hamiltonian of the system, we explore how entanglement generation and evolution depend on the trap frequency, the strength of the interaction, and the number of particles. The study highlights that enhanced coupling and lower temperatures lead to stronger quantum correlations, making such systems promising for quantum information processing and multi-particle quantum technologies.

Background/Introduction:

Mesoscopic systems serve as a bridge between microscopic quantum behavior and macroscopic classical physics. Understanding how multipartite entanglement arises and behaves in such systems is crucial for developing future quantum technologies. The Kratzer potential, widely used in molecular and atomic physics, offers a realistic description of interparticle forces within confined systems.

Objective:

To theoretically analyze how the Kratzer potential and harmonic confinement influence the formation and strength of multipartite quantum entanglement in mesoscopic systems.

Methods: Hamiltonian that includes kinetic, trapping, and interaction terms. Analytical and numerical techniques We model a system of interacting particles confined in a harmonic potential using a total are applied to solve the Schrödinger equation and compute entanglement measures such as concurrence and von Neumann entropy under different system parameters.

Results:

The analysis shows that stronger interparticle coupling and lower temperatures enhance multipartite entanglement. The harmonic confinement stabilizes the correlated states, leading to well-defined quantum correlations that can be tuned by adjusting trap parameters and interaction strength.

Conclusion/Implications:

The findings demonstrate that mesoscopic systems interacting through a Kratzer potential represent viable candidates for implementing controllable multi-particle quantum states. These results provide theoretical insights into the design of quantum devices that rely on collective entanglement and coherent interactions.

Keywords:

Quantum entanglement, Mesoscopic systems, Kratzer potential, Harmonic trap, Quantum information.

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Quantum Computing and AI

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When artificial intelligence (AI) meets quantum computing (QC), a new paradigm of intelligent computation unfolds. Optimization, learning, and physical design converge, forming a self-optimizing ecosystem where software adapts to hardware, and hardware learns from software. AI systems are designed to extract knowledge, infer decision, and detect underlying structures within data. However, QC capitalizes on the lows of quantum mechanics to process information in ways that offer unprecedented computational power, enabling exponentially accelerated and higher-fidelity computation. AI can help make quantum systems more reliable; that is, AI-driven control enhances quantum system robustness and error mitigation. On the other hand, quantum architectures can profoundly augment the computational depth and efficiency of AI models. In the present stage of Noisy Intermediate-Scale Quantum (NISQ) devices, this integration becomes crucial. Therefore, in this work, we present an overview of the transformative potential emerging from the union of these two hyper-disciplines, and their prospective impact across science, biology, physics, and other technologies.

Background/Introduction:

The fusion between artificial intelligence (AI) and quantum computing (QC) signals a shift in computationalthinking. Here, physical design, optimization, and learning work together in real time to build systems in which algorithms are tuned according to hardware, and hardware responds to algorithmic feedback. AI offers mechanisms for autonomous learning and decision-making, and QC takes advantage of the laws of quantum mechanics to handle information beyond classical constraints.

Objectives:

In this work, we present an overview of recent scientific efforts in this field and discuss their collective implications for the development of intelligent quantum technologies. It aims to demonstrate how this integration could advance research in physics, biology, and computational science, and contribute to the emergence of adaptive, self-optimizing quantum systems.

Discussion:

This work shows AI control methods boost quantum device stability through better parameter adjustment and error reduction and adaptive optimization capabilities. Quantum computing serves as an alternative computing system that speeds up AI system development through quick training times and advanced optimization functions and efficient handling of complex high-dimensional data. The alternative computing system of QC enables AI systems to advance through faster training processes and deeper optimization and high-dimensional data processing capabilities. Together, these advantages point toward emerging hybrid AI–quantum architectures capable of iterative adaptation and enhancement.

Conclusion:

This work underscores the profound impact of integrating AI with QC, not only for computation but also for broader scientific discovery. The intersection of AI and quantum principles paves the way for a new generation of co-evolving technologies that may redefine computational modeling, simulation, and applied innovation across disciplines.

Keywords:

Quantum Intelligence, Quantum Computing, AI, Quantum technology.

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Entanglement of spin-1 and spin-0 modes in Bianchi 1 space time universe

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The behavior of entanglement generation in an expanding universe exhibits significant differences between particles of spin-1 and spin-3/2. Recent studies in Friedman-Robertson-Walker (FRW) universe have shown that the entanglement behavior of spin-1 particles resemble those of spins-0, while spin-3/2 particles exhibit behavior similar to spin-1/2 particles. These studies indicate that the absolute values of spin do not play a decisive role in the differences observed in entanglement dynamics, instead, these differences arise from the bosonic or fermionic nature of the particles.

In this work, we extend these analyses by considering the Duffin-Kemmer-Petiau (DKP) equation in Bianchi type-1 universe in (3 +1) dimensions.. By solving this equation we obtain solutions in terms of hyper geometric functions, whose asymptotic behaviors connected through the Bogoliubov transformation technique. Taking into account particles creation processes, we compute the entanglement entropies associated with spin- 0 and spin-1 particles , and compare their behaviors, we analyse how the generated entanglement varies with the parameters characterizing the universes expansion.

Keywords:

Quantum entanglement, DKP equation, Bianchi type-1 universe, entanglement entropy

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κ-Distribution-Based Statistical Theory of Electrostatic Modes in Complex Plasmas with Fluctuating Dust Charge

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In plasma physics, the departure of electron populations from Maxwellian equilibrium and the resulting impact on wave propagation remain of significant interest. This work aims to analyze how κ-deformed statistics, via the κ distribution introduced by Giorgio Kaniadakis to generalize the Boltzmann-Gibbs framework, influence the propagation of electrostatic waves in a plasma composed of electrons, fluid ions, and stationary dust grains with dynamically varying charges. Using the κ-distribution-based statistical theory, we generalize the electron charging-current for dust grains through the orbit motion-limited (OML) model, embed that into the dusty plasma fluid equations, and then apply a reductive perturbation technique to derive a propagation equation of the Korteweg–de Vries–Burger (KdVB) type. Numerical integration using space dusty-plasma parameters reveals that increasing the κ parameter (i.e., stronger deviation from Maxwellian equilibrium) causes the electrostatic shock wave solutions to shift from oscillatory to monotonic form; in the monotonic regime both compressive and rarefactive structures are present, with compressive shocks being enhanced and rarefactive shocks being suppressed as κ grows. These findings imply that the non-extensive deformation of the electron distribution strongly alters the wave dynamics, damping and dispersion balance, and shock profiles in complex plasma. This work provides a theoretical foundation for interpreting wave phenomena in non-thermal plasmas and dusty environments, and offers insights into the role of dust-grain charging under generalized statistics.

Keywords:

κ-distribution, Kaniadakis statistics, dusty plasma, shock waves, variable dust charge

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Bridging Detector-Coupling and Stochastic Theories in Quantum Measurement

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Simultaneous measurement of conjugate observables is restricted by the Heisenberg uncertainty principle. Nonetheless, approximate joint measurements are vital for quantum sensing, and information processing.Two frameworks—Stochastic Quantum Mechanics (SQM) and the Arthurs–Kelly (A–K) detector-coupling model—offer different representations of such measurements. This work investigates whether these frameworks describe equivalent physical measurement processes. An analytical comparison was performed using Gaussian measurement basis states in SQM and explicit detector interactions in the A–K model. Mapping of phase-space variables and dimensional analysis of coupling parameters provided transformation relations between detector readouts and stochastic variables. To validate the analytical results, a numerical simulation was carried out: Gaussian wave functions were used to compute detector probability densities for varying parameters, and fitted balance and scale parameters (b,l) were compared with theoretical values. Model-versus-simulated distributions confirmed the predicted equivalence. The analysis shows that, under a specific detector-balance condition, both models produce identical densities and post-measurement wave functions. This establishes a unified interpretation of stochastic and detector-based quantum measurements. The results offer a foundation for future developments in measurement-aware quantum algorithms, and secure quantum readout systems.

Keywords:
Quantum phase space, Arthurs–Kelly model, Gaussian measurement basis, detector coupling, stochastic measurement formalism

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Mathematical Physics

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Triple differential cross sections for low-energy electron impact ionization of atoms and molecules

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We report Absolute triple differential cross sections (TDCS) for the ionization of water molecules at low impact energies, using the so called 3CWZ/M3CWZ model [1]. In this model, all particles in the continuum are represented by Coulomb waves with variable charges Z(r), and accounts for exchange effects and the post-collision interaction. TDCS for ionization of argon and neon, as wll as the water molecule are reported for varios configurations. The model shows good agreement with experimental data and with other theories, effectively capturing multicenter distortion effects while minimizing computational costs. In our current investigation, we employ the 3CWZ and M3CWZ models to examine the ionization of neon and argon, as well as the orbitals $1b_1 + 3a_1$ of the H_2O molecule, specifically focusing on low impact energies. Our results are presented in Figure 1 as a sum TDCS's of $1b_1$ and $3a_1$ orbitals at low impact energy 65 eV [2], our theoretical results are compared with the MCTDW and M3DW models, showing comparable accuracy to both the available theories and the experimental data.

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Thermal properties of Pauli-oscillator in (anti) de Sitter space

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Using the position-space representation, we present an exact solution of the deformed Pauli oscillator with the (anti)De-Sitter model, where the eigenvalue and the energy Eigen-function are determined by the Nikiforov–Uvarov method. The radial wave functions have been expressed as associated Jacobi polynomials. We also comment on the thermodynamic properties of the system.

Background/Introduction:

There has been growing interest in studying quantum mechanical systems characterized by deformed commutation relations, particularly in curved backgrounds such as de Sitter (dS) and anti-de Sitter (AdS) space-times. In this context, we focus on the analytical treatment of the Pauli oscillator under the influence of an electromagnetic field, when gravitational effects are governed by the Extended Uncertainty Principle (EUP) [1].

Objective:

The aim of this work is to investigate the effects of geometric deformation on non-relativistic quantum systems with spin. We focus specifically on a two-dimensional Pauli oscillator in a deformed space obeying the (AdS) algebra. The findings provide new insights into how such deformations influence the stability, energy spectrum, and thermal behavior of quantum systems, with potential implications ranging from quantum information technologies to cosmological models in theoretical physics.

Results:

The eigenenergies of the system were derived analytically, showing an additional correction term that depends explicitly on the deformation parameter λ. This energy spectrum includes the standard energy levels of the two-dimensional Pauli oscillator, supplemented by a deformation-dependent term. Notably, the correction increases rapidly with the principal quantum number n, indicating a stronger confinement effect as the deformation grows.

Conclusion/Implications:

In this work, we analytically studied the two-dimensional Pauli oscillator under the influence of a deformed algebra in both de Sitter (dS) and anti-de Sitter (AdS) space-times. Using the momentum-space representation of the Extended Uncertainty Principle (EUP) and applying the Nikiforov–Uvarov method, we obtained exact expressions for both the eigenenergies and eigenfunctions of the system. The wave functions are expressed in terms of Jacobi polynomials, and the energy spectrum consists of the standard Pauli oscillator term plus an additional correction induced by the deformation parameter.This correction lifts the degeneracy with respect to the angular momentum quantum number ℓ.

Keywords: Pauli-oscillator, Anti-de Sitter space, Nikiforov–Uvarov method, the Jacobi polynomials

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Battery storage system with Maximum Power Point Tracking for bifacial photovoltaic panels

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This paper presents an intelligent photovoltaic battery storage system with Maximum Power Point Tracking (MPPT) for bifacial solar panels. These PV panels are able to capture sunlight on both sides that leads to generate more power than traditional mono-facial PV modules. In this investigation, the conventional Perturb and Observe algorithm was used to track the maximum power point. Our results demonstrate that the combination of MPPT and the bifacial photovoltaic configuration improved performance and energy yield.

Keywords: Battery storage system, Maximum power point tracking, Bifacial Photovoltaic panels, perturb and observe algorithm.

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Sizing and Performance Prediction of a Photovoltaic Public lighting system powered by a solar panel based on a new CZTSSe absorber under real climatic conditions

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This study presents the sizing and performance prediction of a photovoltaic public lighting system. MATLAB software was used to model and simulate the behavior of the photovoltaic system under real climatic conditions. The parameters of a single solar cell based on a new CZTSSe absorber material were taken from experimental results reported in the literature. The proposed photovoltaic panel consists of 20 CZTSSe based solar cells connected in series. The system was analyzed under the most unfavorable climatic conditions in Constantine city. The results show that the battery reaches its required charge after 9 hours, providing sufficient energy to power an 18 W LED for approximately 15.4 hours. Furthermore, the comparative analysis with a conventional silicon-based device confirms the viability of CZTSSe based solar panel as a low-cost alternative for photovoltaic public lighting systems.

Keywords:
CZTSSe based solar panel, photovoltaic public lighting, MPPT.

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Small amplitude dust-acoustic solitons energy in the presence of Cairns–Gurevich polarization force

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The effect of trapped non-thermal polarization force on low-frequency solitary waves (dust acoustic solitons) is addressed in a collisionless complex plasma. For this purpose, we have firstly redefined the three-dimensional Cairns–Gurevich distribution that describes, simultaneously, the evolution of the energetic ions and those trapped in the plasma potential well, and derived the associated both density and polarization force expressions. The polarization force effects are remarkably modified due to the presence of the trapped non-thermal ions. In particular, we have found that the polarization force magnitude decreases with the increase of ion non-thermality character. Next, the modifications arising in dust-acoustic (DA) solitons and its energy due to the presence of these trapped non-thermal density and polarization force are analyzed. In particular, we have found that the presence of the polarization force leads to an increase in the amplitude and width of DA solitary wave can be propagated in different complex plasma media. Finally, a complementary study on the polarization force effects on the DA energy, associated with both space and experimental dusty plasmas, is also carried out. Our numerical results have shown that more is strong the polarization force more is higher the energy transported by DA solitons.

Background/Introduction:

Since several theoretical works focused on the effects of polarization force on both linear and nonlinear dust acoustic modes in plasmas. Amongst these works, we cite the work of Khrapak et al. [1]. In their analyze, they have found that polarization interaction causes a decrease in the wave phase velocity. Later, Bandyopadhyay et al. [9] showed that, for a given value of Mach number, an increase of the polarization force leads to modification in the amplitude and width of the DA soli-tary waves. Some years later, Mayout et al. [2] studied the modifications arising in the dusty plasma sheath formation due to the presence of polarization forces. They have found that the critical Mach number, beyond which the dusty plasma electrostatic sheath setsin, decreases when the polarization effects increase. F urthermore, the same authors have examined the impact of the polarization force on the energy transported by the DA soliton [3]. In particular, they showed that the DA energy decreases with the increase in the magnitude of the polarization force. More recently, Benzekka and Tribeche [4] have analyzed the combined effect of higher-order corrections and polarization force on the DA soliton. They have found that the departure between the width of the K-dV soliton and the dressed one becomes more important as polarization effects increase. In addition to the above works, some authors have introduced the effects of non-Maxwellian polarization force on the propagation of DA solitary waves .

Objective:

The effects of Gurevich–Cairns polarization force on DA solitary waves and its energy, associated with space dusty plasma.

Conclusion/Implications:

we have investigated the effect of trapped non-thermal polarization force on DA solitary waves and its energy in a collisionless dusty plasma having thermal electrons, negatively charged dust grains, and ions following the Cairns–Gurevich distribution. For this purpose, a three-dimensional Cairns–Gurevich distribution that describes, simultaneously, the evolution of the energetic ions and those trapped in the plasma potential well is

so redefined, and, consequently, both density and polarization force expressions are determined. Our investigation, applied to both space and experimental dusty plasmas, reveals that the effects of the polarization force are significantly modified due to the presence of the trapped non-thermal ions. In particular, we have found that an increase in the ion non-thermal parameter α leads to a decrease in the magnitude of the polarization force. Next, by using the reductive perturbation method, the mK-dV equation has been derived. To show the effect of the polarization force on the DA energy, a comparative study, between experimental and space dusty plasmas, is carried out. Our numerical investigation has shown that more is strong the polarization force more is higher the energy transported by DA solitons. Because of the wide pertinence of nonlinear localized structures in both laboratory and space dusty plasmas , we think that the present findings should help to understand the observations of space plasmas which plainly show the presence of non-thermal and trapped ion populations.

Keywords:

Dust acoustic solitary waves; Cairns–Gurevich distribution function; trapped-non-thermal polarization force; Dust acoustic soliton energy

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Advanced Fault Diagnosis in Bearing: Integrating Discrete Wavelet Decomposition and AI Techniques (SVM with Deep Learning) for Accurate Defect Classification

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This article focuses on the detection of bearing faults by employing a combination of discrete wavelet decomposition (DWD) and artificial intelligence through Support Vector Machine (SVM) approaches. In the field of bearing fault detection and prediction, numerous methods have been explored, but none of these is perfect [1][2]. Many of these methods are beset by issues such as the intricate process of extracting vibratory signals [3]. In light of these challenges, the proposed work harnesses the power of DWD decomposition and SVM to mitigate the limitations encountered in previous techniques and enhance accuracy [4]. The results presented in this paper substantiate the efficacy of the proposed methodology in detecting and classifying bearing faults in induction motors [5].Keywords: Rotating machines, fault diagnosis, bearing defects, Support Vector Machine (SVM), discrete wavelet (DWD) decomposition

Background/Introduction:

This paper is centered around the analysis and classification of various defects in bearings. The approach used combines Discrete Wavelet Decomposition (DWD) with Artificial Intelligence techniques, specifically Support Vector Machines (SVM) along with deep neural network-based web learning, to achieve this analysis and classification.

Objective:

The main objective of this study is to develop and evaluate an efficient methodology for the diagnosis of bearing faults in induction motors by integrating Discrete Wavelet Decomposition (DWD) with Artificial Intelligence techniques, specifically Support Vector Machine (SVM) and deep learning. The aim is to:

- Improve the accuracy of fault detection and classification in rotating machines.

Overcome limitations of traditional signal analysis methods in handling vibratory signals.

- Provide a comparative assessment between DWD, SVM, and deep learning approaches to highlight their strengths and drawbacks in real fault scenarios.
- Contribute to predictive maintenance strategies that enhance the reliability and safety of electromechanical systems.

Conclusion/Implications:

In recent decades vibration analysis has made the monitoring and diagnosis of rotating machinery an effective tool for detecting defects and monitoring their development over time. Various methods of analysis of a vibratory signal are used to improve the monitoring system. By reporting to other analysis techniques vibratory analysis has many advantages.

This paper proposes a comparison between three effectiveness methods (DWT and SVM and Deep network learning) for the detection of defects in induction motors beearing. Which is one of the best and most powerful ways to detect and predict faults in induction motor.

Keywords:
Rotating machines, fault diagnosis, bearing defects, Support Vector Machine (SVM), discrete wavelet (DWD) decomposition

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Study the reduction of short channel effects (SCE) in transistor MOSFET with a new Analytical model

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The intensive reduction in dimensions for a transistor MOSFET at nanoscale ladder imposes significant constraints, in particular to control the short channel effects (SCE). These constraints can degrade the performance of the device. In this work, we have studied the effect of new kind of structure and nanoscale dimensions on performance of MOSFET transistor to face these challenges. An analytical model it is based on an exact solution of two-dimensional Poisson's equation in cylindrical coordinates. The model provides a simple and direct way to calculate subthreshold current (I_{ds}), drain induced barrier lowering (DIBL), subthreshold slope (SS) and the thresh old voltage (V_{th}). which lead to understand the behavior of the device. It is also revealed that new kind structures with specific dimensions are needed to reduce short-channel effects (SCE). The simulation work obtained so far is comparable to that of the literature. We confirm that the analytical models are useful not only for circuit simulations, but also for device design and optimization.

Keywords:

Analytical model, MOSFET, short channel effects (SCE).

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The Chemical Laser: Principles, Operation, and Applications

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Background/Introduction:
Chemical lasers are an advanced technology where coherent light is produced directly by chemical reactions. First demonstrated by Kasper and Pimentel in 1964, they have evolved into high-power laser sources with diverse applications from military to scientific fields.

Objective:
This study aims to explain the operating principles of chemical lasers, particularly the Chemical Oxygen Iodine Laser (COIL), and to analyze their applications across various sectors as well as the associated technical challenges.

Methods:
The approach is based on a detailed literature review, including foundational articles, patents, and technical reports. The operation of the COIL is analyzed in three stages: chemical pumping:production of singlet delta oxygen, amplification
via energy transfer to iodine, and the design of suitable optical cavities.

Results:
Chemical lasers, especially the COIL, deliver megawatt-level power with over 15% efficiency, enabling their use in missile defense, material processing, and spectroscopy. Key deployment challenges include complex logistics, hazardousreagents, and atmospheric beam degradation.

Conclusion/Implications:
While chemical lasers provide unmatched power for defense and industry, their future hinges on overcoming inherent logistical and environmental drawbacks, driving research toward more sustainable and compact alternatives.

Keywords:
Chemical Laser, COIL, Laser applications, Photodissociation,optical gain

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Characterization and simulation of N-Type ion interaction with semiconductor

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In this work, we studied the distribution and the damage induced by the radiation of As+ ions into Silicon targets at energy and to a dose is well known. Ion implantation is a method largely used to fabricate a semiconductor with a shallow junction in the surface target.

The phenomenon induced by the ion implantation was investigated by simulation using the SRIM and CRYSTAL-TRIM code. Several ion implantation parameters, such as projected range, standard deviation and the depth of defects, were estimated with a good accuracy.

To recover the damage induced by the ion implantation and to activate arsenic atoms, annealing treatments were carried out. The samples were analyzed by different experimental techniques such as a four point resistivity measurements, widely used for semiconductors.

For as-implanted samples, an increasing of the resistivity was noticed in the Si layer. After the annealing treatment, a good recovery of defects was obtained. The X-ray analysis was in agreement with electrical measurements. We note that the obtained results were in agreement with literature.

Key word:

interaction ion with matter, ion implantation, arsenic, silicon

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First-Principles and Mathematical Analysis of the Optical Properties of TiO_2 for Photocatalytic Applications

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Titanium dioxide (TiO_2) is a widely used oxide semiconductor due to its high chemical stability, non-toxicity, and strong photocatalytic activity under UV irradiation. Studying the electronic and optical behavior is essential for improving its efficiency in photocatalytic and photovoltaic applications. This study aims to investigate the electronic structure and optical properties of TiO_2 using a first-principles approach. Density Functional Theory (DFT) calculations were carried out using the CASTEP. A Hubbard U correction was applied to Ti 3d orbitals to improve the accuracy of the band gap. The computed band gap (~3.0 eV with DFT+U) indicates a semiconducting behavior, while the optical spectra show strong absorption in the ultraviolet region. These results of mathematical and computational modeling in predicting the photocatalytic performance of oxide materials. The correlation between the calculated band structure and the optical absorption reveals the fundamental mechanisms governing photocatalytic activity. These results confirm that theoretical and computational approaches such as CASTEP .

Keywords:

TiO_2; photocatalytic; UV irradiation; optical properties.

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La Sociophysique en tant que Science Hybride et le Rôle des Modèles de Galam dans la Dynamique de Décision Collective

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Sociophysics is a hybrid field applying concepts and tools from Statistical Physics (e.g., the Ising model) to analyze complex collective social behaviors. This domain's challenging foundation stems from a late 1970s intellectual conflict, where the attempt to extend physical laws to culture was met with strong methodological antagonism.This paper analyzes the pivotal role of Serge Galam's Model in shaping public opinion dynamics. Galam's Model, based on the Local Majority Rule, unveils the Critical Threshold Shift phenomenon, demonstrating how a Minority Opinion can prevail in even-sized groups (Opinion Ties) despite having less than 50% initial support. Validated by simulation and Big Data analysis, Sociophysics provides a robust framework for studying Non-Equilibrium Systems. It stands as a powerful tool for delivering quantitative and kinetic predictions concerning complex socio-economic transformations.

Keywords:
Sociophysics; Statistical Physics; Simulation; Galam's Model; Collective Decision.

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Thomas Fermi regime of neutrons stars at finite temperature

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We present our numerical calculation to study the behavior of neutron stars at finite temperature and in Thomas Fermi limit. This system of BEC is described by the famous Gross-Pitaevskii equation and the term which contains the gravitational contribution is described by Poisson equation that can be solved by iterative processes. Our work combines these two methods in order to study the time evolution of a self-gravitating.

Keywords:
Bose Einstein condensation (BEC); Gross-Pitaevskii equation; Gravitational potential, Poisson equation

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Pair creation in graphene via the Bogoliubov transformation approach in non-commutative phace space

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In this work, we have studied the pair creation of quasiparticles in monolayer graphene by an external electromagnetic field in a non-commutative phace space usig the Bogoliubov transformation between the "in" and "out" states.

Background/Introduction:

At first, the Schwinger effect was studied for a constant electric field [1] More generally, the issue of pair creation was studied for various configurations of fields, such as the electromagnetic field. For example, this problem was treated in the presence of a constant electromagnetic field for both scalar and spinorial particles using the Bogoliubov transformation method. Furthermore, in [2] the author used Schwinger's method for calculating the effective action and the pair production probability for both scalar and spinorial relativistic particles in the presence of a constant electromagnetic field plus a volkov plane wave. He showed that the results for scalar and spinning particles are different by the spin factor. On the other hand, Schwinger pair creation for monolayer graphene in a constant electromagnetic field, and in noncommutative phase space coordinates was studied in [3] using Schwinger method.

Objective:

In this work, we study the creation of quasiparticles in monolayer graphene by an external electromagnetic field and in noncommutative phase space coordinates using the Bogoliubov transformation method.

Conclusion/Implications:

In this workr, we have studied the problem of pair creation of scalar and spinorial relativistic particles from a vacuum by a constant electromagnetic .field in the framework of NC phase space coordinates using the Bogoliubov transformation method.

Keywords:

Graphene, Schwinger effect ,Bogoliubov transformation method, quasiparticles.

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Electron impact ionization of water molecule in the low energy regime.

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Collisions between charged and neutral particles play a fundamental role in atomic and molecular physics. A major area of research focuses on the single ionization of atomic and molecular targets by electron and positron impact known as the (e,2e) process, which provides detailed insight into the behavior of these projectiles during their interaction with the target in the entrance channel, as well as with all resulting particles in the exit channel. Such studies are essential for advancing our understanding of fundamental atomic and molecular mechanisms. The ionization of the water molecule (H_2O) is of particular interest, as water is a vital component of biological systems and plays a key role in numerous physical, chemical, and biological processes. Investigating its ionization dynamics offers valuable information relevant to both fundamental physics and applications in radiation biology and medical physics.

We present a theoretical investigation of the ionization of the water molecule in its ground state by electron impact at low incident energies. Within the framework of mathematical physics, the reaction is described using the M3CWZ model, which relies on detailed mathematical modelling of the continuum states, where each outgoing particle is represented by a Coulomb wave with a position-dependent charge Z(r). The post-collision interaction (PCI) is explicitly and accurately treated. Numerical results are compared with available experimental data and other theoretical models over a broad range of kinematic conditions [1] [2].

Keywords:
Electron, Ionization, Water molecule, TDCS.

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Bound state solutions of screened Coulomb potential under plasma medium

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This study investigates the influence of plasma screening on the non-relativistic behavior of a Positronium through the application of a radial screened Coulomb potential. By accurately solving the Schrodinger equation in spherical coordinates, by using new approach method, we get the self-energy spectrum of our system.

Keywords:

Positronium,Schrödinger equation ,Plasma.

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Determination of the Molar Entropy and Gibbs free energy of the Lithium Dimer (Li_2) Using the Feynman Path Integrals Method

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In this study, the molar entropy and Gibbs free energy of the lithium dimer were obtained using the deformed hyperbolic barrier potential. For this purpose, the Feynman path integral method was used to determine the explicit expression of the energy spectrum, and then the explicit expression of the partition function was derived using the Poisson summation formula. Using the partition function, we calculated the different thermodynamic quantities. Our results for the molar entropy and Gibbs free energy are in very good agreement with the experimental data from the National Institute of Standards and Technology (NIST).

Keywords:
Path integrals, partition function, molar entropy, Gibbs free energy.

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Deformed DKP equation with Dunkl derivative

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In this paper, we presented a study of the two-factor Dunkl-DKP oscillator in the case of spin zero, and using the cartesian coordinates, we obtained in the case of spin zero the eigenvalues of energy and the wave function.

Introduction:

Recently, a great deal of research work has been given to study the effect of deformed algebra in various physics studieds, especially relativistic oscillators. These microscopic phenomena in which spin plays important role in their interpretation this purpose we find DKP oscillator (Duffin ,Kemmer ,Petiau) [1]. and with the advent of the Dunkl [2] have increased interest in its function to solve these various problems due to its structure and impressive results, there has been an increasing number of studies on the Dunkl distortion because it gives additional information in all areas of physics, and the DKP oscillator is considered one of the most attractive of these subjects in terms of results, for example : because of its inversion, it has been used in many physical problems. its gives sufficient information about the integrity of the quantum system to obtain a better and more distinct tuning, several forms of the Dunkl derivative have been presented, Finally a summary.

Conclusion:

In this research, In this research, we examined the two-factor Dunkl-DKP oscillator, and through the Cartesian coordinates, the eigenvalues of energy and the wave function were determined in the case of zero spin.

Keywords: DKP oscillator; Dunkl derivative.

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Analytical Study of Combined Potentials for Selected Diatomic Molecules Using the Path Integral Formalism

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In this research, we present an analytical solution for a combined potential system consisting of the *q*-deformed Hulthén potential and the modified inversely quadratic Yukawa potential, both of which belong to the class of exponential-type potentials. This framework enables the investigation of diatomic molecules through the Feynman path integral approach. Our analysis reveals the effect of the deformation parameter '*q*' on the energy spectrum and the corresponding wave functions. In addition, we evaluate several special cases, and the obtained results show good agreement with previously reported studies.

Keywords:
Path Integral; diatomic molecules; modified inversely quadratic Yukawa potential; q-deformed Hulthén potential; the deformation parameter.

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Entropy of Black Holes in Noncommutative Geometry

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Noncommutative geometry aims to provide a deeper understanding of the theoretical formulation of quantum gravity and serves as a suitable mathematical framework for the study of black holes. In this work, we investigate the thermodynamic properties of black holes in a quantized noncommutative spacetime. The analysis is based on a modification and quantization of the metric in isotropic coordinates, leading to new solutions of Einstein's field equations. Following the approach proposed by S. Solodukhin, our results show that when the quantization effects induced by the noncommutative structure are taken into account, a quantum-type radiation emerges. The general expression of entropy is derived, showing explicit dependence on the number of quantum states and reflecting the combined influence of quantization and noncommutativity on the event horizon. These results offer new insights that may contribute to bridging General Relativity and Quantum Mechanics.

Keywords:
Noncommutative geometry; entropy; quantum gravity; black holes.

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Comparative study and analysis of the Auger transition elements from $_{73}$Ta to $_{83}$Bi

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Background/Introduction:
Because L-shell Auger yields of various elements have numerous uses in physical chemistry and medical research, theoretical, experimental, and analytical methods for calculating these yields are crucial. The Auger yields are critical in developing trustworthy theoretical models for fundamental inner-shell processes. Numerous practical applications, such as elemental analysis using the X-ray emission technique, fundamental research on the atomic and nuclear processes that result in the emission of X-rays and Auger electrons, and dosimetry calculations for medical physics.

Objective: the purpose of empirical calculations is to deduce values of atomic parameters for elements that cannot be measured experimentally or calculated theoretically,deriving new empirical values allows us to compare them with experimental data in order to validate our measurements.

Methods: This research presents new parameters for calculating Auger Decays for targets with atomic numbers Z. We used the mathematical method of polynomial interpolation (least squ
are method) to derive the empirical Auger transition probabilities from the existing experimental data published during the period 1979 to 2003,The database for the a_1-subshell Auger Decays relies on the papers of, Öz [1], Krause [2] and, Özdmir [3].

Results: The obtained results show relatively good agreement with those from other research groups, emphasizing the importance of integrating empirical and theoretical approaches to characterize spectroscopic properties of materials in a coherent way over a while dynamic range. The method used to calculate empirical Auger Decay produced reliable values, which can be integrated into formulas and computer codes for calculating X-ray ionization and Auger Decays.

Conclusion/Implications: The results showed that the empirical method was important for precisely describing the spectral features of materials, and they were in strong accord with other research teams' conclusions. This agreement shows that the learnt method can improve the prediction accuracy.

Keywords: X-ray, Auger transition, Empirical calculation.

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Stability of Falling Liquid Film on Flexible Substrates

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This study investigates the linear stability of a gravity-driven liquid film flowing over a flexible inclined surface using a weighted-residual integral boundary layer (WRIBL) model. The analysis focuses on how wall flexibility influences the onset and nature of flow instability. In the low Reynolds number limits, reduced wall stiffness is shown to destabilize the system. Even when the Kapitza number (Ka) increases meaning surface tension effects become stronger, the short-wave and long-wave instability remains present and is not significantly reduced or suppressed. This suggests that surface tension alone cannot stabilize both wave disturbances, and that wall flexibility is the main driver of this instability. These findings highlight the critical role of wall compliance in triggering and modulating instabilities in thin film flows.

Keywords:
thin film flow, flow instability, flexible substrate, weighted-residual integral boundary layer.

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Using DFT method for investigating physical properties of Double Perovskite La_2MnRuO_6 Alloy

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Background/Introduction:

Double perovskite oxides are at the forefront of materials science due to their vast chemical versatility and rich physical phenomena, making them ideal candidates for next-generation spintronic and optoelectronic applications. This research addresses the need for a comprehensive understanding of the multifunctional properties of La_2MnRuO_6.

Objective: Perform a systematic first-principles investigation of the structural, mechanical, electronic, magnetic, optical, and thermoelectric properties of La_2MnRuO_6 to assess its potential for advanced device applications.

Methods: The study was conducted using density functional theory (DFT) as implemented in the WIEN2k code, which utilizes the full-potential linearized augmented plane-wave (FP-LAPW) method. Structural optimization was performed with the PBE-GGA functional, while the modified Becke-Johnson (mBJ) potential was employed for accurate electronic, optical, and thermoelectric property calculations.

Results: Our calculations predict a stable cubic (Fm-3m) structure with a ferromagnetic ground state for La_2MnRuO_6. The electronic structure reveals a distinct half-metallic character. The material is found to be mechanically stable and ductile, with strong optical absorption in the UV region and a high thermoelectric power factor at elevated temperatures.

Conclusion/Implications:

The results position La_2MnRuO_6 as a promising multifunctional material. Its unique combination of robust half-metallic ferromagnetism, stability, and favorable optical and thermoelectric properties makes it a compelling candidate for the development of advanced spintronic, optoelectronic, and energy-harvesting technologies.

Keywords: Double Perovskite, DFT, Half-Metallicity, Spintronics, Thermoelectric Properties.

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Enhanced Structural, Magnetic, and Magneto-Optical Properties of Fe/Pd(001) Ultrathin Films: Theoretical Study

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Ultrathin magnetic films have attracted considerable attention due to their interfacial and quantum confinement effects, which significantly alter their structural, electronic, and magnetic properties compared to bulk materials. Understanding these effects is essential for developing next-generation spintronic and magneto-optical devices. In this work, we present a comprehensive theoretical investigation of Fe_n/Pd(001) ultrathin films grown pseudomorphically using the density functional theory (DFT) framework with a fully relativistic spinpolarized linear muffin-tin orbital method in the atomic sphere approximation (SPR-LMTO-ASA)[1,2].

Objective: The main objective of this study is to explore the structural, magnetic, and magneto-optical properties of Fe ultrathin films deposited on a Pd(001) substrate and to elucidate the influence of interfacial effects on their behavior. Our computational approach involves total energy optimization, structural relaxation, and magnetic moment analysis for different Fe layer thicknesses, taking into account relativistic spin–orbit coupling effects[3].

Results: The results reveal that Fe atoms form a body-centered tetragonal (bct) structure on the Pd(001) surface, exhibiting an enhanced tetragonality ratio compared to bulk Fe. The interfacial interaction between Fe and Pd atoms leads to significant changes in magnetic coupling, with both intra- and interlayer ferromagnetic ordering observed. The calculated magnetic moments show a pronounced enhancement relative to bulk Fe, primarily due to interface-induced hybridization and reduced dimensionality. Furthermore, analysis of the polar magneto-optical Kerr effect (MOKE) spectra identifies distinct interband transitions responsible for the observed Kerr rotations, providing insight into the optical and magnetic anisotropy of the system[4] These findings deepen the understanding of structure–property relationships in Fe/Pd ultrathin films and highlight their potential for magneto-optical and spintronic applications. The strong coupling between structural distortion, magnetic enhancement, and optical response positions Fe_n/Pd(001) systems as promising candidates for nanoscale magnetic device engineering[5].

Keywords:
Ultrathin films, Fe/Pd(001), Density Functional Theory, Magnetooptical Kerr Effect, Spintronics

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Velocity-Velocity Correlation Function and Transport Processes in Plasma

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An electron gas is a one-component plasma, in which electrons move against a positively charged background to achieve charge neutrality. Transport coefficients are among the most important physical properties studied.They can be expressed as terms of autocorrelation functions, and the Velocity-Velocity Correlation Function (VVCF) is one of the most prominent. Which will be the subject of study in this work. The mathematical statement VVCF was determined based on statistical physics and kinetic theory. It was solved numerically using numerical methods based on the Monte-Carlo method. The values of the Electrical Conductivity Coefficient (ECC) were also determined by this limit of low to medium density. The results emerging from this numerical method were also compared with the results of Spitzer's theoretical method.The comparison showed that the method used in this work is valid in the weak correlation limit, and it also indicated the necessity of adding corrections and modifications, such as introducing the effect of e-e collisions. Overall, the method under study here is a promising and fruitful way to calculate the electrical conductivity coefficient as a start.

Keywords:
Plasma, autocorrelation functions, electrical conductivity coefficient.

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First-principles study of the electronic properties of inorganic perovskite RbPbBr3 and CsPbBr3 for solar cell applications

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Lead halide perovskites have attracted great interest because of rapid improvements in the efficiency of photovoltaics based on these materials. To predict new related functional materials, a good understanding of the correlations between crystal chemistry, electronic structure properties is required First principles calculations by means of the potential linearized augmented plane wave method within generalized gradient approximation (GGA) were carried out for the electronic properties of Main-Group halide compounds RbPbBr3 and CsPbBr3. They have cubic structure and show indirect band gap, the density of states and band gap pressure coefficients are given.The results are compared with previous calculations and experimental measurements, we show that our calculated values compare acceptably well with values reported in the literature.

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Morphology and Structural study of a High Entrop Alloy by Scanning Electron Microscopy

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High entropy alloys (HEAs) represent anovel alloy fabrication concept involving five or more elements in equiatomic or near equimolar ratios. Their unique multicomponent nature leads to the formation of simple solid solution phases rather than complex orbrittle intermetallics, yet their synthesis from elemental powders with differing ductility presents a complex challenge in controlling microstructure and phase formation. This study addresses this by investigating the processing of the model FeCoCrNiMn Cantor alloy via mechanical alloying. Powders were milled for 48 hours, heat treated in the DSC (differential scanning calorimeter) up to 900°C, and sintered at 600°C,X-ray diffraction of the milled powder revealed an anocrystalline mixture of FCC and BCC solid solutions. Subsequent heat treatment stabilized a predominantly FCC structure, while sintering introduced oxide phases and significant grain growth. Scanning electron microscopy of powder illustrated a complex microstructure of flattened aggregates and sharp fragments, indicative of the cyclic competing of cold welding and fracture mechanisms inherent to this ductility-brittleness system. These findings highlight the critical influence of post-milling thermal treatment on the final phase stability and microstructure, underscoring the need to optimize consolidation parameters to prevent contamination and achieve desired properties in HEA systems.

Keywords:

Mechanical alloying, High entropy alloys, Structure, Mechanical properties.

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Interaction configuration in the double ionization of Neon

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The double ionization (DI) of neon by electron impact provides a new approach for electron electron correlation in closed shell atomic systems. In this work, we investigate the DI of neon using the Configuration Interaction (CI) method to model both initial and final state correlations. The total wave function of the neon atom is constructed as a linear combination of multiple electron configurations, allowing explicit treatment of correlation among the 2p electrons, we calculate the fully differential cross sections (FDCS) for a range of kinematic conditions, focusing on the interplay between the shake-off and knock out mechanisms. The CI approach captures both short range dynamic and long range static correlation effects, which are crucial for describing correlated electron emission in neon.

Keywords:
Double ionization, electron correlation, collision theory, atomic

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On new observables in 4D topological gauge-affine gravity

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The realization of a BRST cohomology of the 4D topological gauge-affine gravity is established in terms of a superconnection formalism. The identification of fields in the quantized theory occurs directly as is usual in terms of superconnection and its supercurvature components with the general affine group. Then, by means of a suitable decomposition of the group GL(5,R) with respect to the general linear group GL(4,R), one can easily obtain the enlargements of the fields while remaining consistent with the BRST algebra. This leads to the descent equations, allowing us to build the observables of the theory by means of the BRST algebra. In particular, we discuss the construction of topological invariants with torsion.

Keywords: BRST symmetry, Observables, Descent equations formalism, 4D Topological gauge-affine gravity

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Pair Creation in (1+2)D Coulomb Fields Using the Dunkl-Klein-Gordon Equation

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Scalar particle pair creation in a(1+2)-dimensional Coulomb field is investigat-ed within the framework of the Dunkl formalism. The Dunkl–Klein–Gordon equa-tion is solved exactly, providing analytical expressions for both the angular and radial parts of thewave function. Using the Bogoliubov transformation, we com-pute the pair creation probability along with the associated particle number den-sity. Our analysis reveals that these quantities exhibit a strong dependence on the quantum numberm, the external field strength, and the Dunkl deformation pa-rameter. Remarkably, the Dunkl framework permits pair creation even form=0, highlighting the pivotal role of reflection symmetry in amplifying vacuum instabil-ity.

Scalar particle pair creation in (1+2)-dimensional Coulomb fields is investigated within the framework of the Dunkl formalism. The Dunkl-Klein-Gordon equation is solved exactly, yielding analytical expressions for both the angular and radial components of the wave function. Employing the Bogoliubov transformation, we evaluate the pair creation probability and the corresponding particle number density. The analysis demonstrates that these quantities strongly depend on the quantum number m, the external field strength, and the Dunkl deformation pa-rameter. Remarkably, the Dunkl approach allows pair creation even for m=0, thus under-scoring the crucial role of reflection symmetry in enhancing vacuum instability.

Background/Introduction:

Pair creation in strong external fields is a fundamental prediction of quantum field theory, with the Schwinger mechanism representing the most prominent case. In two-dimensional Coulomb systems, this process is highly sensitive to the field strength and to the symmetries governing the quantum dynamics. The Dunkl-Klein-Gordon (DKG) formalism extends the standard Klein-Gordon equation by incorporating Dunkl derivatives, which introduce reflection operators and defor-mation parameters. This extension provides a consistent framework to analyze pair production phenomena where reflection symmetry plays a central role.

Objective:

The aim of this study is to derive exact analytical solutions for scalar particle pair creation in a (1+2)-dimensional Coulomb potential within the Dunkl formalism, and to determine the pair creation probability and number density through the Bogoliubov transformation.

Methods:

The Dunkl-Klein-Gordon equation is solved exactly by separating angular and ra-dial components. The radial eigenfunctions are obtained in terms of confluent hy-pergeometric functions. The Bogoliubovtransformation is employed to compute transition amplitudes, allowing the evaluation of both pair creation probabilities and particle densities.

Results:

The findings reveal that pair creation probabilities depend explicitly on the exter-nal field strength (V0),the quantum number (m), and the Dunkl deformation pa-rameter ($\mu = \mu 1 + \mu 2$). Unlike the conventional case, the Dunkl approach permits pair creation even for ($m = 0$),emphasizing the crucial role of reflection sym-metry in enhancing vacuum instability. In particular, for ($\mu = 0$), spontaneous pair creation occurs when the critical charge satisfies $Zc>|m|/e^2$.

Conclusion/Implications:

The Dunkl formalism not only reproduces established results but also extends the theoretical understanding of vacuum instability in two-dimensional systems. By embedding reflection symmetry, it enriches the framework of pair creation in quantum field theory. Future directions include extending the analysis to spin-½ particles via the Dirac–Dunkl equation, with the goal of exploring spinor pair cre-ation in external Coulomb fields.

Keywords:
Dunkl formalism, Dunkl-Klein-Gordon equation, Bogoliubov transformation, pair creation, Coulomb potential.

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3CWZ Model Investigation of Ionization by Charged-Particle Impact

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The ionization of argon 3p by positron impact at an incident energy of 200 eV is investigated using the 3CWZ theoretical model.

Background/Introduction:

Ionization by charged-particle impact plays a crucial role in understanding fundamental atomic collision dynamics. While electron-induced ionization has been extensively studied, positron impact remains less explored and presents distinctive interaction features due to the projectile's positive charge.

Objective:

The main objective of this study is to examine the impact of projectile charge (positron versus electron) on the ionization of argon 3p and to evaluate the performance of the 3CWZ model in accurately describing ionization mechanisms at intermediate energies.

Methods:

The Three Coulomb Waves with variable effective charge (3CWZ) model is used, in which continuum states of all particles are represented by Coulomb waves with spatially varying effective charges Z(r). The model accounts for post-collision interaction (PCI) and exchange effects. Triple differential cross sections (TDCS) are calculated for different kinematic conditions and compared with recent experimental data from Dubois and de Lucio [1] and other theoretical predictions.

Results:

The 3CWZ model exhibits very good agreement with experiment and successfully distinguishes the effects of projectile charge (positron versus electron) on ionization behavior.

Conclusion/Implications:

The results confirm that including variable effective charges, PCI, and exchange effects is vital for achieving accurate ionization modeling. This work enhances understanding of charged particle–atom interactions and demonstrates the robustness of the 3CWZ approach in atomic collision physics.

Keywords:

Ionization, positronimpact, 3CWZ model, post-collisioninteraction

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Investigation of electronic and vibrational features of cubic perovskite alkaline tantalite Kx-1NaxTaO3(x=0, 0.25, 0.5)

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Alkaline tantalate $K_{1-x}Na_xTaO_3$ (x = 0, 0.25, 0.5) has attracted considerable attention in recent years due to its interesting photocatalytic properties. Its photocatalytic activity is influenced by several factors, making it an ideal model system for in-depth theoretical investigation. In this work, we present first-principles studies of the structural properties of the cubic ($Pm\bar{3}m$) $K_{1-x}Na_xTaO_3$ phase. The structural and lattice dynamics of these alloys have been investigated using first-principles calculations based on density functional perturbation theory (DFPT) and the virtual crystal approximation (VCA). The variation of the structural parameters, the optical and acoustic phonon frequencies at the high-symmetry points Γ, X, and L, the electronic and static dielectric constants, and the Born effective charges are analyzed as a function of the Na concentration (x).

Keywords:

Perovskite oxides, Photocatalytic materials, Virtual crystal approximation (VCA), DFPT

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Characteristics and Transformations of Dust Acoustic Double-Layers in Plasmas with adiabatically trapped-nonextensive ions using T-Sallis-Gurevich distribution

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The investigation focuses on examining the characteristics of dust acoustic double-layers (DADLs) in the presence of adiabatically trapped-nonextensive ions featuring T-Sallis-Gurevich distribution. Indeed, the ion-density and pseudo-potential expressions are formulated in terms of transcendental functions, allowing for a detailed analysis of Dust Acoustic Double Layers associated with complex plasmas in the presence of non-extensive adiabatically trapped ions. The study then delves into the impact of background ion nonextensivity on key DA-DLs properties. The findings reveal that our plasma model can exhibits both compressive and rarefactive DA-DLs, depending on the nonextensive parameter q. As the value of q increases, the negative DA-DLs reduces in size and eventually transforms into a positive structure. This transformation allows for the existence of compressive DA-DLs. This investigation, prompted by observations in space and laboratory plasmas containing non-Maxwellian particles alongside trapped particles, has the potential to complement and offer fresh insights into previous works on solitary waves in plasma.

Keywords: Dust acoustic waves, Double layers, Tsallis-Gurevich distribution, Nonextensive trapped ions density.

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Analytical High-Temperature Expansion of the 3D Hubbard Model via Many-Body Perturbation Theory

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We employed the divided-difference many-body perturbation theory (DD-MBPT) to investigate the magnetic properties of the three-dimensional one-band Hubbard model, including both nearestneighbor and next-nearest-neighbor hopping amplitudes. This approach provides a systematic and numerically stable framework for evaluating thermodynamic quantities at finite temperature. The contributions of Hugenholtz (Feynman) diagrams were analyzed symbolically and reformulated in terms of divided differences, which greatly simplifies the treatment of Matsubara frequency summations and enables efficient computational implementation. Using this formalism, we computed the coefficients of the grand potential expansion up to the eighth order in both the interaction strength ((U)) and the inverse temperature (β). These high-order expansions allow for a detailed characterization of correlation and magnetic effects in the Hubbard model, providing insight into the interplay between temperature, interaction strength, and electronic structure. The divided-difference representation also enhances numerical accuracy and scalability, making the method suitable for systematic investigations of strongly correlated systems beyond low perturbative orders.

Keywords: Divided differences, Many-body perturbation theory, Hugenholtz vacuum diagrams, Finite temperature

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Electron impact ionization of water molecules: an improved BBK model.

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Triple Differential Cross Sections (TDCSs) are calculated using an improved theoretical model to investigate the dynamics of electron-impact ionization of atoms and molecules. The proposed model is an enhanced version of the BBK approach, in which both outgoing electrons the scattered and the ejected are described by Coulomb waves with variable charges Z(r), instead of a constant effective charge. This fully quantum mechanical treatment extends our previous work, which already showed good agreement with experimental data [1]. Two variants of the model are introduced:

- **BBK2CWZ1**, where the scattered electron experiences an asymptotic charge Zs=1Z_s = 1Zs=1;
- **BBK2CWZ0**, where the scattered electron feels Zs=0Z_s = 0Zs=0, accounting for its higher velocity and the inclusion of the ejected electron in the ionic field.

Calculations are performed for coplanar asymmetric kinematics, and the obtained results are compared with available experimental data. When applied to the ionization of the water molecule [2], both BBK2CWZ1 and BBK2CWZ0 provide TDCS results in very good agreement with experiment, unlike the standard BBK model, which fails to reproduce the observed structures, particularly at large ejection angles. This discrepancy is attributed to strong momentum transfer and recoil effects, where interactions with the residual ion become dominant a regime that remains theoretically challenging.

Keywords:

Ionization ,Electron, TDCS, Water molecule, Coulomb wave, variable Charge

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Standard Model

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Effective Potential and Spontaneous Symmetry Breaking

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In this work, we investigate the possibility of spontaneous symmetry breaking within a scalar field theory reformulated using an auxiliary field (σ). By integrating out the fundamental fields, we derive the effective potential, which contains both logarithmic and arctangent quantum contributions. The analysis focuses on identifying the vacuum structure of the theory: a trivial vacuum at σ=0 or a non-trivial vacuum at $\sigma_0 \neq 0$. The presence of a non-zero minimum indicates the emergence of spontaneous symmetry breaking. Furthermore, the second derivative of the effective potential is studied to determine the effective mass and the stability of the vacuum. This approach allows us to explore the role of quantum corrections in generating symmetry breaking and to specify the parameter ranges that lead to such a phase transition.

Objective:

The objective of this study is to investigate how the auxiliary field σ and the parameter a influence the effective potential, the conditions for symmetry breaking, and the emergence of new phases.

Methode:

In this work, we adopted an analytical and theoretical approach to study the effective potential of the model. The method consists of introducing auxiliary fields, performing functional integration over the fundamental fields; and then carefully computing the result. We applied Feynman parametrization and integral techniques to derive closed-form expression involving logarithmic and arctangent functions. This systematic approach ensures mathematical consistency of the derivation, and allows the final effective potential formula to be analyzed in order to determine the condition for spontaneous symmetry breaking.

Results:

The study revealed that the effective potential, after introducing the auxiliary field and integrating over the fields, strongly depends on the relationship between the effective mass $M^2 = m^2 + \sigma$ and the parameter a. It was shown that the symmetry breaking condition is satisfied when the effective potential becomes negative for certain values, leading to the emergence of a new phase distinct from the ordinary one. This highlights the crucial role of the auxiliary field σ in determining the phase structure, as well as the significant influence of the cutoff parameter Λ on the stability of the theory.

Conclusion:

The analysis of the effective potential confirms that under certain parameter conditions, spontaneous symmetry breaking is possible. The existence of non-zero vacuum expectation values indicates the presence of new phases and an effective mass generation. These results contribute to a deeper understanding of field theory dynamics and quantum phase transitions.

Keywords: Quantum phase transitions, effective potential auxiliary field, spontaneous symmetry breaking.

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Phenomenology of Processes Forbidden at O(Θ) but Allowed at O(Θ2) in the Noncommutative Standard Model

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Noncommutative extensions of the Standard Model (NCSM) provide a framework to probe quantum properties of space-time at high energies. The idea of non commuting coordinates, first introduced by Snyder [1] and further developed through noncommutative geometry and string theory [2], is realized in the NCSM via a noncommutative (NC) parameter Θ. Gauge and matter fields are related to their commutative counterparts through the Seiberg-Witten (SW) map [2,3]. In this work, we investigate the impact of noncommutativity on scattering processes, focusing on corrections at first and second order in the NC expansion. Two representations of Θ are considered; the scattering cross section is then computed in the International Linear Collider (ILC) energy range. At first order, corrections to vertex vanish due to the anti-symmetric structure of Θ, charge conjugation, and momentum symmetry, implying no observable deviations from the SM at O(Θ). At second order, however, NC effects contribute non-trivially, producing modifications in cross sections, angular distributions, and polarization asymmetries. Our analysis demonstrates that while some processes remain unaffected by noncommutativity at leading order, measurable deviations arise only at O(Θ2). These results refine the phenomenological expectations for collider searches, indicating that observable signatures of space-time noncommutativity scale as O(Θ2), thereby enabling constraints on the NC scale ΛNC from precision measurements at future colliders.

Keywords:
Noncommutative space-time, Noncommutativity parameter, Scattering processes.

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Top Quark Transverse Momentum Distribution in Associated tW Production at Hadron Colliders within the Non-Commutative Standard Model

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We present a phenomenological prediction for the transverse momentum distribution of the top quark in associated production at the Large Hadron Collider (LHC) within the framework of the Standard Model (SM).. Upon conducting our calculations for the leading order for both the non-commutative geometry (NCG) and the strong nuclear coupling , the distribution maintains its general shape as in the SM, with deviations in the high region resulting from NCG effects. In the low region, there is a match between the NC distribution and the SM distribution. We also present in our analyses a comparison of the NC distribution with the next-to-leading-order distribution (NLO) in the Standard Model. We observe that it is possible to determine a lower bound for the NCG parameter, beyond which the deviations in the NC distributions become apparent.

Keywords:
Top quark, non-commutative geometry, QCD.

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Higgs Term Contribution to $e^+e^- \rightarrow l\bar{l}$ in The Non-commutative Standard model

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Non-commutative scale parameter Λ_{NC} is a fundamental constant, which characterizes the threshold where non-commutative ffects become relevent, its role can be compared to that of $\hbar$ in conventional quantum mechanics. This work aims to obtain a constraints on this parameter based on the effects du to space-time non-commutativity occurring in leptons pair production in the process $e^+e^- \rightarrow l\bar{l}$ where the electron and positron beams are polarized. This work is an extension of the previous one. This time we take into account the pair production resulting from Higgs boson exchange, which we considered negligible in the previous work. The total crossection and the angular distrubition of the final state are presented at tree level QED calculation and up to the secend order in non-commutative parameters $\theta_{\mu\nu}$ .finally we get a new constraint on Λ_{NC}. The center of mass energy $\sqrt{s}$ is considered to be in the range$300 \rightarrow 500$ GeV and we take into account the case of fully polarised e^+e^- beams because these condition will take place at the future International linear collider (ILC), So our results may be tested.

Keywords:
Standard Model, Non-commtativity, _NC , International Linear Collider.

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Noncommutative Standard Model Effectsin $e^+e^-\to ZH$ Production at TeV Linear Colliders

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Noncommutative geometry elevates space -time coordinates to non-commuting operators, producing testable departures from Standard Model dynamics at TeV energies [1]. Within a Seiberg -Witten map noncommutative Standard Model, we analyze Higgs Z-associated production, $e^+e^- \to ZH$, computing total, and differential cross sections while retaining all orders in the antisymmetric tensor $\Theta_{\mu\nu}$ [2]. The laboratory orientation of $\Theta_{\mu\nu}$ is modeled dynamically by incorporating Earth's rotation. Predictions are presented both instantaneously and as sidereal-time averages across $\sqrt{s}$ and the noncommutative scale Λ_{NC}. Our study reveals a significant suppression of the total ZH cross section for $\sqrt{s} \gtrsim 1$ TeV relative to the Standard Model. The deviation increases as Λ_{NC} decreases and disappears in the commutative limit $\Lambda_{NC}\to \infty$. In addition, noncommutative effects break the flat azimuthal behavior expected in the Standard Model. They generate a characteristic oscillatory φ dependence with distinct peaks and troughs [5]. Because $\Theta_{\mu\nu}$ selects a fixed direction in an inertial frame, Earth's rotation induces a sidereal (diurnal) modulation of both the rate and the angular distributions. This provides a time-dependent handle on the signal. Taken together, energy-dependent suppression, azimuthal anisotropy, and sidereal variation these features constitute complementary probes of space -time noncommutativity [3, 4]. Precision measurements of $e^+e^- \to ZH$ at future TeV-scale linear colliders such as the ILC and CLIC can therefore either reveal such effects or set competitive lower bounds on Λ_{NC}. This sharpens our understanding of potential geometric deformations of space-time at high energies.

Keywords:
Noncommutative Standard Model, Higgs production, e^+e^- collider, cross section, azimuthal asymmetry.

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Cosmology

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Constraints on Chaplygin Gas Models in Modified Gravity from CMB

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The accelerated expansion of the Universe remains a major challenge in cosmology. While the ΛCDM model explains many observations, it suffers from theoretical issues such as the cosmological constant problem. Alternative approaches, including Chaplygin gas and modified gravity, attempt to unify dark matter and dark energy. In this work, we investigate generalized Chaplygin gas models in the framework of modified gravity and confront their predictions with Cosmic Microwave Background (CMB) data. Our analysis shows that these models can reproduce late-time acceleration while remaining consistent with CMB constraints. Distinctive features at large angular scales may help discriminate them from ΛCDM.

Background/Introduction:

The discovery of cosmic acceleration has motivated the exploration of models beyond ΛCDM. Chaplygin gas and modified gravity are two promising candidates.

Objective:

We aim to study the cosmological implications of Chaplygin gas in modified gravity and test their consistency with CMB anisotropy data.

Methods:

The generalized Chaplygin gas equation of state is embedded in a modified gravity framework. Analytical derivations and numerical simulations are used to obtain cosmological evolution and CMB predictions, which are compared with Planck data.

Results:

The models reproduce the late-time acceleration while remaining consistent with CMB constraints. Distinctive features in the low-ℓ multipole region may allow these scenarios to be distinguished from ΛCDM.

Conclusion/Implications:

Chaplygin gas in modified gravity offers a viable alternative to ΛCDM, unifying dark matter and dark energy while preserving agreement with observations. Future large-scale surveys could provide further tests of their validity.

Keywords:

Chaplygin gas, modified gravity, Dark energy, CMB power spectrum, Cosmology.

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Noncommutativity and the Thermodynamic Phase Structure of Black Holes

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In this work, we study the thermodynamic properties of the noncommutative Schwarzschild Anti-de Sitter (AdS) black hole, obtained by incorporating the effects of spacetime noncommutativity into the classical Schwarzschild AdS geometry [1]. From the modified metric, we derive the corresponding Hawking temperature [2] and evaluate the Helmholtz free energy to analyze the phase structure of the system. Our results show that, for specific values of the noncommutative parameter Θ and a fixed cosmological constant, the free energy exhibits the characteristic swallowtail behavior, which is a clear indication of a two-coexistance phase transition between small and large black hole passing through a new intermediate phase. When the noncommutative parameter approaches its critical value, the swallowtail structure disappears and the system undergoes a second-order phase transition marked by an inflection point in the free energy curve. This reveals the coexistence of two types of phase transitions first- and second-order depending on the strength of the noncommutative effects. Such behavior closely parallels that of charged AdS black holes and Van der Waals fluids [3], confirming that noncommutativity enriches the thermodynamic phase structure and induces critical phenomena similar to those found in extended black hole thermodynamics. These findings align with earlier studies of noncommutative-inspired black holes. [4,5]

Keywords:
non-commutative geometry, Schwarzschild AdS black hole, thermodynamic proprieties.

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Dark Energy within the Pseudo-Complex General Relativity

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The Pseudo-Complex General Relativity (pc-GR) formalism, utilizing pseudo-complex coordinates ($\boldsymbol{I^2 = 1}$), automatically introduces terms into the system that are interpreted as dark energy. This energy provides a repulsive, anti-gravitational effect for high central mass density, effectively halting the collapse of a large stellar mass.
The important result is that the collapse into an event horizon at is avoided and no singularity is formed. Consequently, black holes do not exist in this framework; the resulting massive compact object is viewed as a gray star.
I investigate the modified pc-Schwarzschild solution (for a static mass), treating the dark energy component as a fluid, and present corrections implied by charged (Reissner-Nordström) and rotating (Kerr) gray stars. The theory naturally incorporates a minimal length parameter $\boldsymbol{l}$.
Finally, I discuss several key predictions that distinguish pc-GR from standard GR, including the modified orbital speed of a mass in a circular orbit around a gray star, which offers a possible method for experimental verification, as well as deviations in gravitational redshift and the perihelion shift of Mercury.

Keywords:
Pseudo-Complex General Relativity, Dark Energy, Gray Stars, Event Horizon.

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Logarithmic correction to the entropy and the non-commutative correlation of Schwarzschild black hole radiation

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In this work we investigate the entropy of the Schwarzschild black hole (BH) and the statistical correlations of black hole radiation in a non-commutative (NC) framework, using several methods to explore the effect of this geometry. First, we obtain NC corrections to the BH entropy using Bopp's shift, the star product, and an NC gauge-theory approach, and we compare the results. We find that the usual area law is violated in this geometry. Using the first law of BH thermodynamics, we derive a logarithmic correction to the NC entropy: the correction from Bopp's shift is the smallest, whereas the NC gauge theory yields the largest correction. The form of the NC corrections is similar to those found in other quantum-gravity models, with prefactors related to the Planck length. Finally, we use these expressions to study how non-commutativity (and the different computational methods) affect the statistical correlation between successive particle emissions from an NC Schwarzschild BH. In all three methods (Bopp's shift, star product, and gauge theory) non-commutativity reduces the statistical correlations between successive emissions, an effect analogous to the presence of a potential well in quantum mechanics. The gauge-theory method produces the smallest correlations compared to the other approaches, suggesting that NC gauge theory is a particularly sensitive framework for studying quantum-gravity effects on BH physic.

Keywords:
Non-commutative geometry; Schwarzschild black hole, Black hole entropy; Quantum gravity; Statistical correlation

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Time delay in matched exterior and interior Kottler solutions

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We extend the study of gravitational lensing to photons traversing the lens mass, modeled as a uniform-density fluid described by the interior Kottler (Schwarzschild–de Sitter) solution smoothly matched to the exterior Kottler region. An analytic expression for the time delay is derived, allowing the interior contribution to be explicitly isolated relative to the vacuum Kottler case. This correction is found to systematically enhance the total time delay, an effect corroborated by numerical evaluations for astrophysically relevant lenses at both galaxy and cluster scales. These results underscore the importance of accounting for the interior lens structure in accurate modeling of strong lensing time delays.

Background/Introduction Gravitational lensing time delays provide key insights into both cosmological expansion and the internal structure of astrophysical lenses. Standard treatments based on the exterior Schwarzschild–de Sitter (Kottler) metric neglect interior mass contributions, an assumption invalid for extended systems such as galaxies and clusters where light can traverse the lens. This study revisits lensing in a *matched* interior–exterior Kottler geometry that consistently incorporates a cosmological constant.

Objective To derive analytic expressions for the gravitational time delay of photons propagating through a uniform-density fluid sphere matched to an exterior Kottler spacetime, isolate the interior correction relative to the vacuum case, and quantify its astrophysical impact for galaxy- and cluster-scale lenses.

Methods The analysis constructs a smooth junction between the interior and exterior Schwarzschild–de Sitter solutions and integrates null geodesics across both regions. Using first-order expansions in the compactness parameter, analytic formulas for the deflection angle and travel-time difference are derived. Numerical evaluations are then performed for representative galaxy ($r_B = 25$ kpc) and cluster $r_B = 250$ kpc) configurations with $\Lambda = 10^{-52}\ \mathrm{m}^{-2}$.

Results An explicit expression for the total time delay $\Delta\tau \simeq \Delta\tau_{ex} + 4GM\sqrt{(1-\Lambda r E^2/3)}E_{in}$ is obtained, where E_{in} represents the interior correction. This term systematically increases the total delay relative to the exterior Kottler value. Numerically, for galactic lenses with $M \simeq 1.8\times10^{11}\ M_\odot$, the enhancement reaches 80–100 days, while for cluster lenses with $M \simeq 1.8\times10^{14}\ M_\odot$, the increase amounts to 1.7–2.3 years.

Conclusion/Implications The matched Schwarzschild–de Sitter treatment reveals that interior mass distributions significantly amplify strong-lensing time delays—by up to about 70%—relative to exterior-only models. Accurate modeling of extended lenses therefore requires inclusion of the interior Kottler region. The framework provides a relativistically consistent bridge between idealized point-mass and extended-fluid lenses, and it can be extended to dynamical cosmological backgrounds and causal interior structures.

Keywords: Gravitational lensing, Schwarzschild–de Sitter spacetime, interior Kottler solution, time delay, cosmological constant

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Lensing in matched exterior and interior Kottler solutions

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We analyze gravitational lensing in a matched Kottler spacetime with cosmological constant Λ, where a uniform-density fluid sphere described by the interior Kottler solution is smoothly joined to the exterior Kottler region. We derive an analytic expression for the deflection angle of light rays traversing both regions, isolating the corrections induced by the interior mass distribution relative to the vacuum Kottler case. The interior terms systematically reduce the bending angle and tangential magnification while enhancing the radial one, leading to a scale-dependent effect on the total magnification. Numerical evaluation shows a mild amplification for galaxy lenses and a demagnification for clusters, reflecting the contrast between compact and diffuse configurations. The induced Λ-contribution from the interior corrections further reduces the bending, but only slightly, consistent with its role in the vacuum Kottler case. These results demonstrate that lensing observables retain a measurable imprint of interior structure in SdS-like lenses, crucial for refining realistic strong-lensing models.

Background/Introduction: Gravitational lensing probes both local matter distributions and cosmic geometry. While the exterior Kottler (Schwarzschild–de Sitter) metric models point-like lenses, real galaxies and clusters have extended interiors. The study addresses how finite-size structure and the cosmological constant Λ modify standard lensing predictions.

Objective: To derive analytic expressions for light deflection and magnification in a matched Kottler spacetime—where a uniform-density interior is smoothly joined to the exterior SdS region—and to quantify the observable impact of interior structure and Λ.

Methods: The matched interior–exterior Kottler metric is constructed exactly and expanded to first order in compactness. Light geodesics crossing both regions are integrated analytically to obtain deflection and magnification formulas. Numerical evaluations are performed for galaxy and cluster parameters to compare interior-corrected and pure exterior SdS predictions.

Results: Interior corrections systematically *reduce* the bending angle and tangential magnification while *enhancing* the radial one. The total magnification shows a mild amplification for compact galaxy lenses and a demagnification for diffuse clusters. The Λ-dependent term slightly decreases the bending, consistent with its effect in the vacuum SdS case.

Conclusion/Implications: Lensing observables retain measurable imprints of interior structure, producing scale-dependent signatures in magnification. These results refine strong-lensing models by bridging idealized point-mass and extended astrophysical lenses, with implications for interpreting galaxy–cluster lensing and Λ effects in cosmological contexts.

Keywords: Gravitational lensing, Schwarzschild–de Sitter spacetime, interior Kottler solution, cosmological constant, strong lensing

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Fundamental aspect of gravitational waves

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We investigate the gravitational waveforms generated by perturbed extreme mass ratio inspirals (EMRIs) under the influence of an outer supermassive black hole (SMBH). Using the method of osculating orbits in Schwarzschild spacetime, based on the relativistic orbital evolution equations of Pound and Poisson, we model the orbital evolution of a small compact object around a massive black hole subjected to an external perturbation. The gravitational waveforms are computed through a second-order source-free integration method that numerically solves the Regge–Wheeler and Zerilli equations in the time domain using finite difference schemes and jump conditions at the particle's worldline. Our results show that the presence of an external massive body induces measurable phase shifts in the emitted gravitational waves, which become more significant over time. These perturbations, while initially indistinguishable from the unperturbed waveform, produce temporal deviations that could serve as observable signatures in future space-based detectors such as LISA. This study highlights the potential importance of environmental and third-body effects in the modeling and detection of realistic EMRI signals.

Background/Introduction:

model a gravitational wave of an EMRI perturbed by a third outer body.

Objective:

model the effect of a thord body on the motion of an EMRI and obtain it's waveform

Methods:

We apply the method of osculating orbits in Schwarzschild spacetime using the relativistic orbital evolution equations. calculate the gravitational waveforms of our perturbed EMRI using the second order source-free integration method for black hole perturbations to resolve the Regge-Wheeler and Zerilli (RWZ) wave equations, designed for integration in time domain.

Results:

we found waveform pattern of EMRI's perturbed by outers bodies

Conclusion/Implications:

the outer body influence plays an important role in shaping the GW forms. The wave spectrums are not going to be perturbed at the same rate depending on their initial conditions. EMRI's are generally accompanied by a stars dust background, that are going to perturb the binary geodesic as well as the probable nomadic SMBHs, we expect for EMRI's detections a bunch of perturbed waveforms.

Keywords:

Gravitational waves, three body system, perturbation theory

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Probing the neutrino-antineutrino asymmetry through space-time noncommutativity

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A new mechanism based on space-time noncommutativity has produce anisotropy and an axial-like interaction,yielding leptonic asymmetry for fermionic partricles propagating in a noncommutativity curved FRW universe, As a byproduct, an analytical expression of this asymmetry for ultra-relativistic particles, such as neutrinos,is derived explicitly.Constraints and bounds from the cosmological parameters are also discussed.Space-time noncommutative geometry (NCG) has emerged as an intriguing framework with potential implications for particle physics and cosmology (1),(2). It presents opportunities for addressing cosmological questions byproviding a natural framework for investigating the physics of the early universe.In conclusion, our study uncovers an innonative mechanism that harnesses the noncommutativity of space-time to elucidate the enigma of matter-antimatter asymmetry. This endavor highlights the intricate interplay between NCG parameters, the equation of state parameter, and the neutrino-antineutrino asymmetry, which in turn contributes to the overall understandingof cosmological and reveal new dimensions in our understanding of the universes intricate dynamics.

Keywords :
Noncommutative geometry-modified theories of gravity-leptogenesis

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Implication of scalar field in relativistic stars

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The study of scalar fields in the context of relativistic stars has gained significant attention due to their potential implications in modified theories of gravity, dark matter models, and the late-time acceleration of the universe. In this work, we investigate the influence of a minimally or non-minimally coupled scalar field on the structure, stability, and observable properties of compact stellar objects such as neutron stars and boson stars. By solving the Einstein field equations coupled with a scalar field and an appropriate equation of state, we explore how the presence of scalar fields alters mass-radius relations, tidal deformabilities, and maximum mass limits. Particular emphasis is placed on scalar-tensor theories and models with spontaneous scalarization, which predict observable deviations from general relativity in strong-field regimes. Our results suggest that scalar fields can lead to significant modifications in stellar configurations and provide testable predictions for future gravitational wave and astrophysical observations.

Theoretical Chemistry

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Impact of a single impurity of 3d series on the structural, electronic and magnetic properties of Ag_8 cluster

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This study presents the optimized structures of silver octamer clusters doped with 3d transition metal atoms (Sc-Ni), in their neutral and charged species. Density functional theory calculations, within the generalized gradient approximation for exchange and correlation, were employed to evaluate the stability of the clusters and to examine the effects of doping on their electronic and magnetic properties. All optimized geometries exhibit three-dimensional configurations, with the do-pant atom encapsulated at the center of the cluster and coordinated by surround-ing silver atoms. The enhanced binding energies observed in the doped systems suggest that the insertion of transition metal atoms improves the structural stabil-ity of the Ag8 cluster. The results indicate a general thermodynamic stabilization upon doping. Furthermore, the reduced HOMO-LUMO gaps in clusters doped with Ti, V, and Mn point to potentially favorable optical properties. The calculat-ed magnetic moments range from 0 to 4 μB, with significant values observed for Ti, V, Cr, Mn, Fe, and Co (1.30, 2.78, 4.12, 4.07, 2.89, and 1.50 μB, respectively), highlighting the magnetic diversity introduced by these dopants.

Background/Introduction:

This study is part of research on the structural, electronic, magnetic and optical properties of nanostructured artificial materials (free or supported clusters, surfac-es, etc.) based on transition metals and/or semiconductors. Objective: What is the effect of inserting a 3d transition metal atom into a silver octamer cluster on its structural, electronic and magnetic properties?

Methods:

We performed electronic structure calculations within the framework of density functional theory using the Vienna ab-initio simulation package (VASP), which employs a plane-wave basis set to describe valence electrons [1]. Exchange-correlation effects were treated using the generalized gradient approximation with the Perdew-Burke-Ernzerhof functional [2]. Ultrasoft pseudopotentials for silver and 3d transition metal atoms (Sc-Ni), as provided in the VASP distribution, were used in simulations [3]. The plane-wave cutoff energy was set to 450 eV. Clusters were placed in cubic supercells with a side length of 15 Å, large enough to elimi-nate interactions between periodic images. Calculations were carried out at the Γ-point of the Brillouin zone. Energy convergence was set to 10^{-6} eV, and the force

convergence criterion was 10-3 eV/Å. To identify the ground-state structures, we explored multiple initial geometries and employed the conjugate gradient algo-rithm for structural optimization [4]. The relative stability of different isomers was assessed by comparing total energies for various magnetic configurations. Local magnetic moments on individual atoms were evaluated using Bader charge analysis [5]. To ensure accurate treatment of charged systems, both dipole and quadrupole corrections were applied.

Results:

According to the obtained results, the insertion of a single transition metal atom into the silver octamer cluster significantly modifies its geometric and symmetry properties, promoting the emergence of three-dimensional configurations.The adsorption of impurity atoms results ina notable increase in the binding energy of doped clusters over the pure silver cluster, contributing to greater structural stabil-ity, especially with Sc, Ti, Co, and Ni dopants.The doping of Ag8 cluster with Sc, Ti, V, Cr, and Mnatoms significantly enhances its reactivity, indicating improved resistance to reduction. In contrast, doping with Fe, Co, and Ni results in lower stability;suggesting a diminished ability to maintain the cluster's structural stabil-ity during redox processes.Doping with Fe atoms notably enhances the stability compared to other dopants. Conversely, doping with other 3d transition metals generally decreases the clusters' stability during the oxidation process, indicating a greater susceptibility to oxidation.The presence of Sc, Ti, V, and Cr dopants in the silver octamer reduces the HOMO-LUMO gap, indicate potentially enhanced optoelectronic properties.The total magnetic moments of the doped clusters vary between 0 and 4 μB. The dopant atoms generally retain their local magnetic mo-ments within the non-magnetic silver host, except for Ni, whose magnetic mo-ment is completely quenched. Notably, significant local magnetic moments are maintained for the 3d dopants, particularly Cr, Mn, Fe, and Co.

Conclusion/Implications: Findings suggest that inserting a 3d transition metal atom into a silver octamer cluster significantly enhance its structural, electronic and magnetic properties. The mixed clusters hold promise for applications in various technological do-mains, particularly in optoelectronics and spintronics.

Keywords:

Spin-polarized calculations, Silver, 3d impurities, Binary clusters, Electronic and magnetic properties.

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Local magnetic properties of 3d and 4d impurities in silver hexamer cluster

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The magnetic properties of Ag6X clusters, where X ranges from Sc to Ni and Y to Pd, have been investigated using the density-functional formalism. We have found that the behavior of magnetic moments of binary clusters is similar for doping with 3d and 4d impurities. Large magnetic moments are observed of 3d dopants Ti, V, Cr, Mn, Fe, Co (1.64, 2.98, 4.82, 4.76, 3.62, 1.72), compared to 4d dopants Zr, Nb, Mo, Tc, Ru, and Rh (1.18, 2.50, 3.61, 3.36, 2.23, 1.12), respectively. Therefore, the magnetic moments of 4d elements are small with respect to the 3d elements. The magnetic moments of doped clusters range from 0 to 6 . Density of states analysis show that there are more complicated interactions acting in clusters to affect the local magnetism of the impurities; the interactions of the Ag6-spd orbital with X-pd orbitals play a crucial role on the overall magnetism of the clusters.

Background/Introduction: This study forms part of a broader investigation into the structural, electronic, magnetic, and optical characteristics of nanostructured artificial materials relevant to advanced technologies.

Objective: We compared the effects of inserting a 3d and 4d transition metal atoms into a silver hexamer cluster on its magnetic properties, and identified the hybridization between the impurity's atomic orbitals and those of the surrounding silver atoms.

Methods: Density functional theory simulations were performed using the Vienna Ab initio Simulation Package (VASP). The interactions between valence electrons and ionic cores were described using the projector augmented-wave method [1]. The exchange-correlation functional was treated within the generalized gradient approximation, using the Perdew-Burke-Ernzerhof parametrization [2]. A plane-wave cutoff energy of 450 eV was employed to ensure convergence of the total energy. Since the studied systems are finite clusters, Brillouin zone was restricted to the Γ point. To eliminate interactions between periodic images, each cluster was placed in a cubic supercell of side 15 Å. Structural relaxations were carried out using the conjugate gradient algorithm, with convergence thresholds of 10-6 eV for the total energy and 10-3 eV/Å for atomic forces [3]. All calculations were spin-polarized, and Bader charge analysis was employed to extract both total and local magnetic moments from the spin density distribution [4].

Results: One of the most distinctive features of the doped clusters is their magnetic behavior. In fact, a single atom doped into small clusters affect considerably his magnetic properties. In this work, we show that the insertion of a 3d and 4d impurity in a non-magnetic host silver cluster, lead to magnetic doped clusters especially when doping with Cr, Mn, Fe and Mo, showing the highest magnetic moments.

The results indicate that the local magnetic moments of the impurities increase progressively in the sequences Sc < Ti < V < Cr and Y < Zr < Nb < Mo, while they decrease along the sequences Mn > Fe > Co > Ni and Tc > Ru > Rh > Pd. The total magnetic moments of the doped clusters are either identical to the local moments of the impurities (as observed for V, Ni, and Pd), slightly reduced (as in the cases of Co, Tc, Ru, and Rh), or enhanced (notably for Sc, Ti, Cr, Mn, Fe, Y, Zr, Nb, and Mo), suggesting different hybridization between the impurity atomic orbitals and those of the surrounding silver atoms, as the dopants are embedded within the host cluster structure. To gain insight into the interactions between the X impurity and the host cluster that govern the resulting magnetic moment, we analyzed the partial density of states for the impurities, for the Ag6 host, as well as the total density of states for the doped clusters. The imbalance between the spin-up and spin-down components of the density of states reflects the presence of a local magnetic moment. This asymmetry is particularly pronounced in clusters doped with V, Cr, Mn, Fe, Nb, Mo, Tc, and Ru, indicating spin polarization and significant contribution of the impurity states to the overall magnetism of the system. Several sharp peak overlaps are observed between the partial density of states of the Ag6 cluster and those of the impurities. For instance, pronounced superpositions of the Ag6-spd orbitals with the d orbitals of doped atoms are localized at specific energies: -0.66, 0.76, 1.62, and 2.23 eV for Ag6V; -1.04, -0.28, 1.62, and 3.31 eV for Ag6Cr; -3.48, -0.33, 0.45, and 1.61 eV for Ag6Mn; -3.75, -1.98, -1.25, -0.33, and 1.48 eV for Ag6Fe; -0.51, -0.21, 0.82, 1.74, and 2.27 eV for Ag6Nb; -0.47, 0.02, 1.39, and 2.21 eV for Ag6Mo; -4.69, -2.81, -0.46, 0.57, 1.04, and 1.37 eV for Ag6Tc; and -4.33, -1.11, -0.29, and 1.28 eV for Ag6Ru. Additionally, sharp peak overlaps between the pd orbitals of the Ag6 host and the p orbitals of Mn (2.16 eV), Fe (2.38 eV), and Ru (3.33 eV) are also observed. Consequently, Ag6V (3), Ag6Cr (6), Ag6Mn (5), Ag6Fe (4), Ag6Nb (3), Ag6Mo (4), and Ag6Tc (3) exhibit the highest total magnetic moments within the series of doped clusters. In contrast, clusters such as Ag6Sc, Ag6Ni, Ag6Y, and Ag6Pd display non-magnetic moment, with perfectly overlapping spin-up and spin-down densities of states, signifying the absence of exchange splitting. These results clearly demonstrate that the local magnetic moments of the impurities and the total magnetic moments of the doped clusters are primarily governed by the hybridization between impurity-pd and host cluster-spd orbitals.

Conclusion/Implications: In summary, our study reveals that the magnetic properties of silver hexamer clusters doped with different transition metal impurities are strongly influenced by the hybridization between the impurity's p and d orbitals and the spd orbitals of the silver host. Clusters doped with V, Cr, Mn, Fe, Nb, Mo, Tc, and Ru exhibit notably high magnetic moments, correlated with distinct asymmetries in density of states. In contrast, doping with elements such as Sc, Ni, Y, and Pd result in non-magnetic clusters due to the lack of exchange splitting. These findings emphasize the critical role of electronic interactions at the atomic scale in tailoring the magnetic behavior of doped clusters, with potential implications for nanoscale magnetic devices and spintronic applications.

Keywords:

Simulation, Cluster, Impurity, Hybridization, Magnetism

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Density functional theory (DFT) investigation of calcium oxynitride phosphate (Ca_2PO_3N) at ambient pressure

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We present a study of the physical properties of Ca_2PO_3N. To our knowledge, aside from their synthesis and structural properties, the fundamental physical properties of Ca_2PO_3N have not yet been studied, either experimentally or theoretically. Ca_2PO_3N was synthesized by Alexey Marchuke et al. [1] in 2015. The purpose of this work is to investigate the structural, elastic, and electronic properties of Ca_2PO_3N at ambient condition using first-principles calculations based on the DFT+PP-PW approach, as invoked by the Cambridge serial total energy package (CASTEP) program [2]. We have applied the On The Fly Generated (OTFG) ultrasoft pseudopotential together with the Perdew-Burke-Ernzerhof adapted for solids (PBEsol) of the generalized gradient approximation (GGA) exchange-correlation function [3]. Ca2PO3N crystallizes in the orthorhombic structure with space group Pnma (No. 62) [4], where the conventional unit cell contains calcium cations, which typically coordinate with the phosphonitridate anion (PO_3N). . The optimized lattice parameters are found to be in good agreement with experimental data [1]. The study of elastic constants is useful in understanding the structural stability and the mechanical properties. The elastic constants indicate weaker resistance to unidirectional compression compared to shear deformation for this compound, which satisfies the mechanical stability criteria. Using the Voigt-Reuss-Hill (VRH) method [5], the bulk modulus (B), shear modulus (G) Young's modulus (E) and Poisson's ratio (σ) are also calculated. The band structure of Ca2PO3N indicates that it has a direct band gap(G-G) of 4.004 eV, which is considered a wide gap. A direct band gap allows for efficient electron transitions between the valence and conduction bands without requiring a change in k-point. This property is advantageous for optoelectronic applications, such as light-emitting diodes (LEDs) and photodetectors, as it facilitates strong light absorption and emission. Our future work will focus on studying this compound under high pressure and temperature.

Keywords: structural properties, elastic properties, electronic properties, ab initio study, Oxonitridophosphates

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Reactivity Analysis of Aminopolycarboxylic Acids: A DFT Approach Using Dual Descriptors and Molecular Electrostatic Potential

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Aminopolycarboxylic acids (APCs) are widely recognized as effective ligands for the capture of heavy metals, thereby offering a promising ecological strategy via chelation. Nevertheless, a deeper understanding of their intrinsic reactivity with these heavy metals is still required. This study utilized Conceptual Density Functional Theory (DFT) [1] to elucidate the reactivity of a series of APCs (EDTA, EDDS, EDDM, EDDG, CDTA, and IDS) by identifying their main reactive sites. Dual Descriptors (DD) [2] and Molecular Electrostatic Potential (MEP) [3] were applied to localize these specific sites on each APC molecule. The analysis successfully identified key atoms and sites favorable for nucleophilic and electrophilic attacks. These results provide valuable information on the reactivity patterns of APCs, which is essential for understanding their heavy metal complexation mechanisms and thus guiding the rational design of more effective and selective chelating agents for environmental remediation.

Keywords:
APCs, reactivity, DFT, DD, MEP

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DFT and TD-DFT Study of a New Schiff Base Ligand

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Schiff bases, or imines, are organic compounds containing a carbon–nitrogen double bond (C=N). First reported by Hugo Schiff [1], these molecules have attracted considerable attention due to their ability to form metal complexes and their potential applications in catalysis, medicinal chemistry, and functional materials. Schiff bases are widely used in the pharmaceutical industry, particularly in the synthesis of various biologically active compounds such as antibiotics, antiallergic, antitumor, and antifungal agents [2–3]. These applications are not limited to the laboratory scale but have also been extended to the industrial level, making Schiff bases one of the most widely explored innovative systems in various research fields [4]. Since their discovery, these compounds have drawn the attention of researchers across multiple scientific fields, owing to their exceptional structural, electronic, and optical characteristics.

The main objective of this work is to theoretically investigate the electronic and optical properties of a new Schiff base compound, denoted as L1: 6-methyl-2-oxo-3-[1-(p-fluoroimino) ethyl]-2H-pyran-4-olate. Our study aims to determine and confirm the most stable form of these compounds, which can exist in two main tautomeric forms: the keto-amine and the phenol-amine forms. In this work, the density functional theory (DFT) was employed using the B3LYP and BP86 functionals with the 6-31G basis set. The time-dependent DFT (TD-DFT) method, implemented in the Gaussian 09 program, was used to characterize the excited electronic states and to identify the origin of the optical transitions. his study highlights the significant potential of Schiff bases as active materials in organic photovoltaic devices, owing to their low cost, chemical and thermal stability, and strong ability to efficiently absorb solar radiation.

Keywords:
Schiff Bases, DFT, TD-DFT, photovoltaic, Gaussian 09.

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Étude théorique par DFT des propriétés structurales et électroniques de polymères donneur-accepteur à base de DPP et d'isoindigo.

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Les polymères donneur-accepteur, tels que ceux à base de diketopyrrolopyrrole (DPP) et d'isoindigo (IGT)[1], sont des matériaux prometteurs pour les semi-conducteurs organiques en raison de leurs hautes performances optoélectroniques.
Cette étude vise à comprendre l'influence de l'agrégation moléculaire sur la géométrie, la distribution des charges et les propriétés d'absorption optique de ces systèmes. Une investigation théorique a été menée à l'aide de la théorie de la fonctionnelle de la densité (DFT) avec le logiciel Amsterdam Density Functional (ADF). Les modèles monomères, dimères et trimères des unités DPP et IGT ont été optimisés. Les caractéristiques de transfert de charge ont été évaluées par analyse de population de Mulliken, et les profils d'absorption UV-Vis ont été simulés par DFT dépendante du temps (TD-DFT). Nos calculs démontrent qu'augmenter la longueur de conjugaison provoque un déplacement bathochrome (rouge) des spectres d'absorption et modifie les profils de distribution des charges. Ces résultats théoriques sont en accord avec les observations expérimentales du comportement à faible bande interdite de ces polymères. Ces résultats offrent une compréhension fondamentale au niveau moléculaire des interactions électroniques qui déterminent les performances des semi-conducteurs organiques à haute mobilité émettant dans le proche infrarouge. Cette étude fournit ainsi des indications précieuses pour la conception rationnelle de nouveaux matériaux organiques pour l'optoélectronique.

Mots clé :
Polymères donneurs-accepteurs ; DFT ; TD-DFT ; absorption UV-Vis ; agrégation moléculaire.

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Synthesis, Structural Characterization, and Theoretical Study by DFT and TD-DFT Methods of New Schiff Bases

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Schiff base compounds are multifunctional molecules that play a significant role across various scientific and industrial domains [1–3]. They have been employed as dyes, pigments, corrosion inhibitors, thermostable materials, and catalysts [3, 4], as well as in medical applications, including antifungal, anticancer, and antibacterial agents."

We are interested in the synthesis of a new Schiff base compound DTE, The structure of the compound was determined by Xray diffraction, IR and UV. The theoretical study deals with the calculations, mainly made by means of the functional theory of the density DFT, and time-dependent (TDDFT), the calculations allowed to determine the electronic properties these methods showed their efficiency in the calculations of the molecular structures, reactivity indices, the dipole moment, polarizability and vibration frequencies. UV-visible absorption spectra gives values in excellent agreement with the experimental data. The theoretical calculations obtained, allowed me to confirm their character as DYE sensitizer for their use in organic photovoltaic cells.

Keywords:
Schiff base, DFT, TD-DFT, Dye-senstitizer, X-ray diffraction

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Étude Ab Initio des Propriétés du Composé Intermétallique $FePd_3$

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Our study presents an in-depth theoretical analysis of the structural, electronic, and thermal properties of the intermetallic compound FePd3 in the L12 and D022 configurations, considering both non-magnetic (NM) and ferromagnetic (FM) states. This research was performed using the first-principles FP-LAPW (Full-Potential Linearized Augmented Plane Wave) method, incorporating the PBE-GGA approximation to treat exchange-correlation effects. The calculated results for lattice constants (a, c), the bulk modulus (B), and its derivative (B') show good agreement with existing theoretical and experimental data. Energetic analysis confirms that the FM-L12 phase is the most thermodynamically stable. Furthermore, the electronic band structure analysis clearly reveals the compound's metallic nature. Finally, the mechanical investigation confirms that FePd3 exhibits ductile behavior, satisfying the established criteria: its Pugh's ratio (B/G) is greater than 1.75, its Poisson's ratio exceeds 0.26, and its Cauchy pressure is positive.

Keywords:
FePd3, DOS , L12 , DFT, ductile

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Ab Initio Insights into the Mechanical Behavior of Niobate–Tantalate Double Perovskites for Sustainable Energy Technologies

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The mechanical behavior of the cubic niobate–tantalate double perovskite **Li_2NbTaO_6** was investigated using first-principles calculations within the density functional theory (DFT) framework based on the full-potential linearized augmented plane wave (FP-LAPW) method. Niobate–tantalate perovskites have recently attracted increasing attention due to their thermal stability and multifunctional characteristics, making them promising candidates for high-temperature and energy-conversion technologies. However, their elastic and mechanical features remain poorly understood. In this context, the present study aims to evaluate the mechanical stability, elastic anisotropy, and thermal robustness of **Li_2NbTaO_6** to provide a clear understanding of its lattice response under stress. The optimized structure retains the cubic double-perovskite symmetry with corner-sharing BO_6 octahedra. The computed elastic constants (C_{11} = 365.6 GPa, C_{12} = 77.8 GPa, C_{44} = 102.9 GPa) satisfy Born's stability criteria, confirming the compound's mechanical soundness. The derived bulk, shear, and Young's moduli (B = 172 GPa, G = 116 GPa, E = 286 GPa) indicate a dense and rigid framework resistant to both volume and shear deformations. A negative Cauchy pressure (−24.5 GPa) together with a Pugh's ratio of 1.48 and Poisson's ratio of 0.22 classify **Li_2NbTaO_6** as a brittle material with partial covalent bonding. The Zener anisotropy factor (A = 0.70) reveals moderate elastic anisotropy, while the Kleinman parameter (ζ = 0.30) suggests limited internal strain flexibility. The estimated melting temperature of approximately 2730 K reflects excellent thermal endurance and lattice cohesion at elevated temperatures. Overall, these results demonstrate that **Li_2NbTaO_6** combines high lattice rigidity, brittle mechanical character, and strong thermal resistance, highlighting its potential for high-temperature optomechanical and energy-harvesting applications. The theoretical findings provide a valuable foundation for future experimental synthesis and mechanical optimization of niobate–tantalate double perovskites.

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and shear deformations. A negative Cauchy pressure (−24.5 GPa) together with a Pugh's ratio of 1.48 and Poisson's ratio of 0.22 classify **Li_2NbTaO_6** as a brittle material with partial covalent bonding. The Zener anisotropy factor (A = 0.70) reveals moderate elastic anisotropy, while the Kleinman parameter (ζ = 0.30) suggests limited internal strain flexibility. The estimated melting temperature of approximately 2730 K reflects excellent thermal endurance and lattice cohesion at elevated temperatures. Overall, these results demonstrate that **Li_2NbTaO_6** combines high lattice rigidity, brittle mechanical character, and strong thermal resistance, highlighting its potential for high-temperature optomechanical and energy-harvesting applications. The theoretical findings provide a valuable foundation for future experimental synthesis and mechanical optimization of niobate–tantalate double perovskites.

Keywords:

Li_2NbTaO_6, mechanical stability, DFT, elastic properties, thermal resistance

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In Silico Elucidation of the 5-HT1A Receptor Affinity for Annona Muricata Alkaloids via DFT and Docking.

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Background/Introduction:
Annona muricata (Graviola) is traditionally used for its antidepressant properties, linked to its alkaloid affinity for 5-HT1A receptors. This study evaluates the activity of alkaloids annonaine, nornuciferine, and asimilobine on the 5-HT1A receptor to predict their potential biological activity.

Methods:
We combined Density Functional Theory (DFT/B3LYP) to calculate chemical reactivity descriptors (HOMO-LUMO gaps) and molecular docking to assess binding affinity to the 5-HT1A receptor (PDB ID: 7e2y).

Results/Conclusion:
DFT calculations showed high stability (HOMO-LUMO gaps 4.51–5.36 eV). Docking revealed strong, favorable binding for all compounds (BE between -8.11 and -8.85 kcal/mol). Nornuciferine exhibited the best affinity (K_iC=324.13 nM), primarily driven by π−π stacking and π-Cation interactions. These findings suggest promising serotonergic activity, supporting the traditional use of *Annona Muricata* for mood disorders.

Keywords:
Annona Muricata, Alkaloids, 5-HT1A, DFT, Molecular Docking.

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DFT Study of (E)-1-[-2-(4-fluorophenyl) Diazan-1-ylidene] Naphthalen-2(1H)-one (4-FPDN)

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To understand the conformation of the title compound, we performed Density Functional Theory (DFT) calculations using the B3LYP functional with the 6-311++G (d, p) basis set, implemented in Gaussian 09 [1]. The study provides insights into the electrostatic potential (ESP) distribution [2], as well as the visualization of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO). the Localized Orbital Locator (LOL), and the Electron Localization Function (ELF) were also analyzed. Visualization and analysis were carried out using Multiwfn [3] and VMD Studio [4].

Keywords:

DFT, ESP, HOMO, LUMO, ELF, LOL.

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Unveiling Hidden Mechanical Signatures in the Double Perovskite Li 2 NbTaO 6 : A First-Principles Exploration

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The mechanical behavior of the cubic niobate–tantalate double perovskite Li 2 NbTaO 6 was investigated using first-principles calculations within the density functional theory (DFT) framework based on the full-potential linearized augmented plane wave (FP-LAPW) method. Niobate–tantalate perovskites have recently attracted increasing attention due to their thermal stability and multifunctional characteristics, making them promising candidates for high-temperature and energy-conversion technologies. In this context, the present study aims to evaluate the mechanical stability, elastic anisotropy, and thermal robustness of Li 2 NbTaO 6 to provide a clear understanding of its lattice response under stress. The optimized structure retains the cubic double-perovskite symmetry with corner-sharing BO_6 octahedra. The computed elastic constants (C_{11} = 365.6 GPa, C_{12} = 77.8 GPa, C_{44} = 102.9 GPa) satisfy Born's stability criteria, confirming the compound's mechanical soundness. The derived

bulk, shear, and Young's moduli (B = 172 GPa, G = 116 GPa, E = 286 GPa) indicate a dense and rigid framework resistant to both volume and shear deformations. A negative Cauchy pressure (−24.5 GPa) together with a Pugh's ratio of 1.48 and Poisson's ratio of 0.22 classify Li 2 NbTaO 6 as a brittle material with partial covalent bonding. The Zener anisotropy factor (A = 0.70) reveals moderate elastic anisotropy, while the Kleinman parameter (ζ = 0.30) suggests limited internal strain flexibility. The estimated melting temperature of approximately 2730 K reflects excellent thermal endurance and lattice cohesion at elevated temperatures. The theoretical findings provide a valuable foundation for future experimental synthesis and mechanical optimization of niobate–tantalate double perovskites.

Keywords:

Li 2 NbTaO 6 , mechanical stability, DFT, elastic properties, thermal resistance

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Relativistic DFT Investigation of Uranium(VI/V) Complexes: Electronic Structure and Redox Properties

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This work presents a comprehensive theoretical study, based on relativistic DFT, of a series of uranium complexes of the type $Cp_2U(=N–Ar)X$, where X represents functional ligands with σ- and/or π-donor character. Although the crystal structures of some of these compounds are known, no computational analysis has been reported to date. Our objective is to understand the relationships between their electronic structure, redox behavior, and the nature of the metal–ligand interactions involved.
We performed calculations incorporating relativistic effects, spin–orbit coupling, and solvent interactions, using the ZORA/COSMO+SO method implemented in the ADF code. This approach accurately reproduced the experimental redox potentials ($-E_1/_2$), establishing a strong linear correlation with the calculated electron affinities (EA), with a correlation coefficient R^2 greater than 0.97.
Beyond interpreting experimental data, our study leverages the predictive power of DFT to investigate the redox properties of complexes that are either unknown or have not yet been isolated. This series of compounds, synthesized by Kiplinger's group, provides an ideal framework for testing and validating our theoretical protocol, thanks to the wealth of available structural and electrochemical data.

Keywords: Redox potential, Electron affinity, DFT, ZORA, Uranium complexes

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Relativistic DFT Investigation of Uranium(VI/V) Complexes: Electronic Structure and Redox Properties

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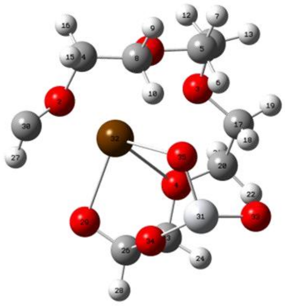
In recent years, the optical capabilities of polymer composites have dominated the marketplace for applications in optoelectronic and energy devices. Supercapacitors, lightemitting displays, optical waveguide sensors, and organic photovoltaic cells are a few examples of the applications of the optical behavior of composites. We try to create smart materials capable of self-healing, changing shape or color depending on conditions, or storing and releasing energy. In the current study, we have calculated the electronic properties such as energy band structure and spectroscopy properties of the $BaTiO_3$ perovskite material and $BaTiO_3$/PEG nanocomposite. DFT and TD-DFT calculations are shown to provide an excellent cost-effective computational approach for the treatment of the excited states of these materials.



$BaTiO_3$/PEG optimized molecule for CAM/B3LYP DFT calculation

Keywords: TD-DFT, Absorption spectrum, $BaTiO_3$/PEG, polymer

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Theoretical Investigation of a Newly Synthesized Azo-Based Organic Material for Photovoltaic Applications

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The synthesis of new organic materials for photovoltaic cells, with an active layer based on organic semiconductors, represents a significant innovation. The present study focuses on determining the structural and electronic properties of a newly synthesized azo material, with the chemical formula $C_{18}H_{18}Cl_2N_2$ and the acronym AZ1. Particular emphasis is placed on its molecular structure to understand the photovoltaic structure-activity relationship of this material.

First, theoretical calculations using density functional theory (DFT), implemented with the Gaussian 09 software, were performed to model the molecular system composing the azo material studied. The geometric parameters (interatomic distances, valence angles, dihedral angles) obtained previously from structural resolution using X-ray diffraction data are compatible with the results generated by molecular optimization using B3LYP/6-31G (d, p).

These calculations are primarily carried out to determine the photovoltaic properties of the material under consideration by studying the charge transfer between the azo molecular structure, type D–π–A, and tetracene, a reference donor material. This charge transfer mechanism between the two materials is determined by the localization of molecular orbitals (HOMO and LUMO), the energy gap value (Eg) and the molecular electrostatic potential surface (MEP). The photovoltaic performance of the analyzed material is interpreted through the open circuit voltage (VOC), the fill factor (FF) and the energy conversion efficiency (PCE).

Keywords: Photovoltaic, semiconductor, azo, DFT, charge transfer.

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AI and Others

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Automated Anomaly Detection in Solar PV Panels using Deep Learning for Enhanced Maintenance

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The escalating global demand for sustainable energy has positioned solar photovoltaic (PV) systems as a pivotal component of future power generation infrastructure. However, ensuring their sustained optimal performance necessitates robust and efficient maintenance protocols. Conventional inspection methods are frequently characterized by high labor intensity, extended durations, and considerable operational costs, thereby impeding the overall efficiency and reliability of PV installations. This paper introduces an advanced AI-driven methodology aimed at automating the crucial processes of inspection and maintenance for solar panels. We detail the development and rigorous training of a sophisticated image classification model, leveraging state-of-the-art deep learning techniques. This model is meticulously designed to precisely identify various performance-hindering anomalies, including but not limited to dust accumulation, micro-cracks, and more significant breakages, with demonstrated high accuracy. The ultimate vision involves seamlessly integrating this intelligent diagnostic tool with autonomous robotic cleaning and repair systems, thereby facilitating fully self-sufficient solar farm management. This proposed framework promises substantial reductions in operational expenditures and system downtime, concurrently enhancing the energy yield and contributing significantly to the overarching objectives of sustainable and reliable energy provision.

Keywords:
Artificial Intelligence, Solar Energy, Predictive Maintenance, Deep Learning, Computer Vision, Anomaly Detection.

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Analysis and Optimization of Methane Production in Anaerobic Bioreactors by Artificial Intelligence

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Amid current energy and environmental challenges, biomass emerges as a promising renewable energy source, convertible into methane-rich biogas via anaerobic digestion. However, the inherent biological complexity and fluctuating operational conditions of this process present significant challenges for accurate prediction of methane production. This study proposes the application of Artificial Intelligence techniques, specifically Artificial Neural Networks, to analyze operational data and enhance methane production prediction. An AI model was developed using a comprehensive dataset to model this process. The model was successfully trained and tested, demonstrating strong and reliable predictive performance in capturing the complex relationships between operational variables and yield levels. A graphical user interface was also developed to facilitate the practical application of the model. This research highlights the potential of Artificial Intelligence as a valuable tool for enhancing the efficiency and supporting the sustainability of bioenergy production operations.

Keywords:
Biomass, Anaerobic Digestion, Methane, Artificial Intelligence,

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Machine Learning and Artificial Intelligence in the Analytical Study of Soft Gluon Emission in QCD at the LHC

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Soft gluon emission is a fundamental aspect of Quantum Chromodynamics (QCD) at the Large Hadron Collider (LHC), governing the infrared structure of scattering amplitudes and influencing precision phenomenology. In the eikonal approximation, multi-loop soft gluon calculations reveal complex color and kinematic correlations whose analytical treatment becomes rapidly intractable beyond a few loops. Traditional symbolic methods, while rigorous, face combinatorial and algebraic limitations. Recent advances in machine learning (ML) and artificial intelligence (AI) provide new avenues to overcome these challenges. By training models such as symbolic regression, graph neural networks, and transformer architectures on exact results up to five loops, AI systems can identify hidden symmetries, infer recurrence patterns, and predict compact analytical forms for higher-loop configurations. These approaches preserve gauge and color consistency while significantly reducing symbolic complexity. The integration of AI with theoretical QCD represents a promising direction for automating multi-loop computations and deepening our understanding of the algebraic structure of soft gluon radiation at the LHC.

Keywords:
Soft gluon, Antenna function, Machine learning

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AI-Based Prediction of Sodium Layer Dynamics for Laser Guide Stars optimizations

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Background/Introduction:

Adaptive optics systems in modern ground-based telescopes depend on sodium laser guide stars (LGSs) to correct for atmospheric turbulence and enhance image resolution. The performance of these LGSs is highly influenced by the mesospheric sodium layer, whose density varies due to altitude, temperature, and atmospheric dynamics.

Objective:

This study aims to develop a predictive model for the mesospheric sodium density using machine learning (ML) methods, providing an approach to improve the real-time calibration and brightness optimization of LGSs in adaptive optics systems.

Methods:

We used long-term observational data sodium lidar collected between 2010 and 2024. The dataset includes altitude-resolved sodium density, neutral temperature, and wind profiles in the 80–110 km region. Several ML algorithms were evaluated, including Random Forest, Gradient Boosting. Model performance was assessed through comparative analysis and feature importance evaluation.

Results:

Ensemble models achieved the highest predictive accuracy, showing strong agreement between predicted and observed sodium density profiles across diverse mesospheric conditions.

Conclusion/Implications:

The results demonstrate that ML-based sodium density prediction offers a reliable method for anticipating LGS brightness fluctuations, enabling more efficient adaptive optics calibration in real time. This approach supports the development of optimized observing strategies for next-generation telescopes such as the European Extremely Large Telescope (E-ELT).

Keywords:

Adaptive optics, laser guide star, mesospheric sodium, machine learning.

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A theoretical study of growth behavior and properties evolution of small Germanium cluster doped

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The different properties of H-doped germanium clusters are systematically studied by means of first principles computations on the basis of the density functional theory (DFT) approach. The doping H atom largely participates to strengthen the Ge13 cluster stability by increasing the binding energie . The various explored clusters possess a total spin magnetic moment going from 0 to 1μB. Introduction: Semiconductors are of great importance in electronic devices, optoelectronics, and solar cell applications. Doped germanium is the most widely used semiconductor in this field. The study of the optical properties of doped Germanium clusters can contribute to research in the field of materials used for optoelectronics and solar cells. Objective: We are trying find candidate materials that can match, or better, materials used in optical detectors and sources. Methods: The clusters geometries were optimized using DFT implemented in the SIESTA package. This program employs pseudopotentials and uses localized orbitals. The self-consistent field (SCF) computations were performed with a convergence criterion of 1x10-4 a.u. for electronic energy. We used the generalized gradient approximation (GGA) of Perdew and Zunger and of Perdew, Burke, and Ernserh (PBE) for the exchange correlation energy. With respect to the polarization function, we utilized a double ζ (DZ) basis for Germanium and H atom with150 Ry cutoff energy.

Keywords:
Germanium clusters, density functional theory, Binding energies, Magnetic properties. **References:**

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