Faculté des Sciences Aïn Chock

Département de Physique

Moroccan day of Quantum Information and Quantum Technologies

Moroccan Network of Quantum Information
Réseau Marocain de l'Information Quantique

25 Décembre 2024, Casablanca

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Pr. Driss Benchekroun	**UH2C, Casablanca**
Pr. Aniss Said	**UH2C, Casablanca**

Objectif de la manifestation

L'objectif principal de cet événement est de permettre aux chercheurs spécialisés dans les technologies quantiques, l'information quantique, la physique des hautes énergies-physique des particules, ainsi que les matériaux et nanomatériaux, de se rencontrer et d'échanger sur les avancées récentes dans leurs domaines respectifs. Cette réunion constituera également une occasion de discuter des nouvelles tendances, des avantages et des défis liés au développement des technologies basées sur les principes de la physique quantique au Maroc.

Thèmes de Recherche

- Information Quantique et Optique Quantique
- Corrélations Quantiques et Codes Quantiques
- Nanomatériaux et Applications Quantiques
- Technologies Quantiques et batteries quantiques
- Physique des Hautes Energies-Physique des Particules
- Machine Learning et Calcul Quantique
- Circuits Quantiques, Cavités QED et Systèmes Ouverts
- Métrologie Quantique et Simulation Quantique
- Physique des Matériaux et physique de la Matière condensée
- Physique Nucléaire et astrophysique
- Sécurité de l'Information Quantique

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Abdellah Sbiri	FSAC, Casablanca
Fatima Zahra Ahlaf	FMPC, Casablanca

Conférences Plénières

Structures de recherche de la Faculté des Sciences Ain Chock de Casablanca

Driss Benchekroun[1]

[1]Laboratory of High Energy Physics and Condensed Matter, Faculty of Sciences Ain Chock, Hassan II University, Casablanca, Morocco – Maroc

Résumé

La faculté des Sciences Ain Chock de Casablanca (FSAC) compte actuellement quinze laboratoires de recherche répartis entre les cinq départements de l'établissement. Ce nombre sera réduit à onze laboratoires lors de la période d'accréditation 2025-2028.

Les activités de recherche de la FSAC s'inscrivent aussi bien dans les thématiques fédératrices nationales (eau, énergies renouvelables, IA, biotechnologies …) que dans des axes de recherche fondamentale. Les travaux de recherche réalisés au sein de la FSAC sont couronnés par la soutenance d'une centaine de thèses de doctorat chaque année.

Les activités de recherches de la FSAC liées à la physique quantique sont diverses et concernent principalement :

- La modélisation en chimie (ou chimie théorique),
- La microélectronique et les nouveaux matériaux,
- La physique de la matière condensée,
- L'information quantique,
- La sécurité informatique et le quantum computing.

Seconde révolution quantique et défis futurs des sciences et technologies de l'information

Daoud Mohammed[1,2]

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[2]Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, I-34151 Trieste, Italy

Résumé

Le prix Nobel de physique 2022 a distingué le Français Alain Aspect, l'Américain John F. Clauser et l'Autrichien Anton Zeilinger pour leurs expériences sur l'intrication quantique et ses applications. L'intrication est un type de corrélation bien spéciale qui existe entre particules à l'échelle microscopique. Elle n'a pas d'analogue classique. C'est une propriété qui fait qu'on ne peut pas dans un système à plusieurs particules attribuer des propriétés individuelles à chaque particule et toute description l'ensemble des particules ne peut se faire que globalement. Les recherches expérimentales sur cette propriété étrange du monde physique à l'échelle microscopique remonte aux années 1960 quand l'Américain John Clauser a réalisé une expérience montrant l'existence de ce type de corrélations quantiques entre photons. Ces corrélations, de nature purement quantique, ne peuvent être comprises à l'aide des outils et principes de la physique classique. En 1983, le Français Alain Aspect affine ces expériences et montre le caractère non local de la mécanique quantique qui autorise l'intrication ou l'entrelacement entre photons. L'autrichien Anton Zeilinger a réalisé des expériences qui exploitent l'intrication pour implémenter des protocoles de téléportation et communications quantiques. Les travaux de ces trois lauréats du prix Nobel 2022 ont ainsi balisé le chemin de nombreuses applications de l'intrication dans divers domaines comme la cryptographie quantique, la métrologie quantique, la simulation quantique, l'informatique quantique,…. Aussi, depuis quelques années est en train de se préparer une seconde révolution de la physique quantique. Beaucoup de projets sont en cours d'expérimentation dans les coulisses des laboratoires à travers le monde et nul doute ses travaux de recherches apporteront des résultats qui révolutionneront le domaine des technologies de l'information. Notre présentation concernera les récents développements et les défis de l'information quantique et ses applications dans le domaine du traitement et du stockage de l'information.

Morocco's Contributions to High-Energy Physics and Beyond: From Fundamental Discoveries to Real-World Applications

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Abstract

Morocco's growing contributions to High-Energy Physics (HEP), with a focus on our involvement in major international collaborations such as ATLAS at CERN, KM3NeT, and ANTARES. These endeavors showcase the country's active participation in cutting-edge research aimed at probing fundamental questions about the universe. In the ATLAS experiment, our team has contributed to the analysis of proton-proton collisions, advancing the understanding of Standard Model processes and beyond, while exploring novel detector technologies and calibration techniques. In KM3NeT and ANTARES, we have been instrumental in neutrino detection, contributing to the exploration of astrophysical neutrino sources and advancing neutrino-based multimessenger astronomy. Furthermore, we emphasize the development of HEP-inspired applications beyond fundamental research. These include advancements in machine learning techniques derived from HEP data analysis, their integration into AI-driven projects such as AI4TB, and the application of detection and imaging technologies in medical physics and radiation safety.

Innovative Smart Materials for Energy Harvesting Applications

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Abstract

The demand for portable electronic devices and wireless detectors has increased with the growth in the production of microelectronic and mechanical systems (MEMS) in the past decade. Currently, the development of intelligent materials has been recently used for numerous applications such as electrochromic systems for perfectly improved performance. The potential of piezoelectric composite and the smart textiles has been investigated for many areas such as sensing applications. Due to various their excellent properties these materials are becoming widely attractive especially in applications intended energy harvesting. Firstly, the aim is to enhance the intrinsic proprieties of these materials in order to gain a deeper understanding of their functional properties, and to enhance their performances for a better using in the electromechanical and radio frequency conversion in order to develop the micros systems miniaturized, autonomous, communicating and totally flexible. The second part focuses, on the one hand, on the using of flexible composite films with different BCZT/Ps contents in electromechanical conversion and which allows to capture environmental vibrations and converts them into electrical energy. And on the other hand, on the development and conception a compact super-wideband flexible textile antenna which It operates over an extremely broad frequency range. Owing to its simple topology, compact size, super-wideband behaviour, and high gain, endorse its suitability for low-power requirement applications in the real world.

Keywords: Piezo-nanoparticle; Smart composite, electromechanical conversion; Alltextile antenna, RF conversion, energy harvesting.

Non-Markovian effects on the performance of a quantum Otto refrigerator

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Abstract

Thermodynamics plays an important role in science and engineering. It was introduced at the start of the industrial revolution and applied to the design of a wide variety of large scale useful devices, from refrigerators to solar cells. Nowadays, technological progress is increasingly miniaturized at the nanoscale and in the quantum regime, where thermal fluctuations compete with quantum fluctuations. Moreover, quantum thermal machines have been a focus of active research in the last decade for describing fundamental concepts at the nanoscale. Hence, it is important to study how thermodynamic quantities like work, heat and power can be significantly attributed to the familiar processes of quantum information theory. Afterwards, we move towards the development of autonomous systems to study different thermodynamic quantities. We investigate the non-Markovian effects of the reservoirs used to extract cooling from an autonomous refrigerator machine.

Machine Learning and Its Role in Quantum Computing

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Abstract

Machine learning (ML) has emerged as a powerful tool for extracting insights from data, solving complex problems, and optimizing processes across various domains. This talk will introduce the foundational concepts of machine learning, including supervised and unsupervised learning, in a manner accessible to those unfamiliar with the field. Building on this foundation, we will explore how ML intersects with quantum computing, showcasing its applications in optimizing quantum hardware, correcting errors, and enhancing quantum algorithms. Through a combination of reviews and novel perspectives, this presentation aims to highlight how the synergy between ML and quantum technologies could drive advancements in quantum information science and beyond.

Communications Orales

1) Information Quantique

Dynamics of Quantum Correlation in a Two-qutrit Heisenberg XXZ Model with Heitler-London and Dzyaloshinskii-Moriya Couplings

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Résumé

This study investigates the dynamics of quantum coherence and entanglement in the spin-1 Heisenberg XXZ model. Particularly, we examine the effects of the Heitler-London coupling and the Dzyaloshinskii-Moriya interaction. By utilizing tools from quantum information theory, we explore the concept of quantum correlated coherence and negativity. Our results show intrinsic decoherence leads to a decay of both correlated coherence and negativity. Interestingly, we find that a small value of the Dzyaloshinskii-Moriya interaction can significantly enhance coherence and entanglement. Various factors influence the system dynamics, including the initial state, anisotropy parameter, and the coupling distance between spins. We show that, by fixing the anisotropy parameter, we can easily recover the isotropic Heisenberg models XX and XXX. Ultimately, our findings highlight that the system maintains a coherent temporal evolution despite decoherence.

Geometric measure of quantum correlation and coherence in the ising-XYZ diamond chain under an external magnetic field

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Abstract:

This presentation explores the geometric measure of quantum correlation and coherence in the Ising-XYZ diamond chain, which comprises both Ising and Heisenberg spin particles subjected to an external magnetic field. The first step involves calculating the reduced density matrix using the transfer matrix approach (TMA). Subsequently, quantum correlations and coherence in the Ising- XYZ diamond chain are quantified through Negativity (N), local quantum uncertainty (LQU), and the $l1$ norm of coherence $Cl1$. The study investigates the influence of thermal noise and various system parameters, including the xy-anisotropy α, the Heisenberg interaction Γ among interstitial sites, Ising spin exchange $J1$, and the magnetic field strength, on the dynamics of quantum resources within the system. The results reveal that temperature and magnetic field adversely affect these quantum properties. Conversely, higher values of the xy-anisotropy parameter enhance quantum correlation and coherence, thereby alleviating the negative impact of temperature. This research provides valuable insights into the behavior of quantum resources within this system.

Keywords: Ising-XYZ, Heisenberg chain, Negativity, Local quantum uncertainty, $\boldsymbol{l1}$ norm of coherence, Diamond chain.

Geometry of two mode squeezed thermal gaussian state

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[1] University Ibn Tofail, Faculty of Sciences, Kenitra, Morocco

Résumé

In the present work, we tackled the problem of evaluating the volume of Gaussian physical states. The relevance of considering Gaussian states is twofold: first, Gaussian states are the most commonly experimentally used CV states. Second, Gaussian quantum states are represented in the phase space picture of quantum mechanics as proper the volume of Gaussian states by information geometry, hence Gaussian quantum states are the volume of Gaussian states by information geometry coming from Wigner functions in phase space. Thereby, dealing with The volume of Gaussian states by information geometry, Information Geometry appears as a natural and unifying approach for evaluating volume of quantum states.

Révélation des corrélations non-classiques, de la cohérence quantique et contrôle de l'incertitude de mesure dans un modèle de spin XY-Γ à deux qubits

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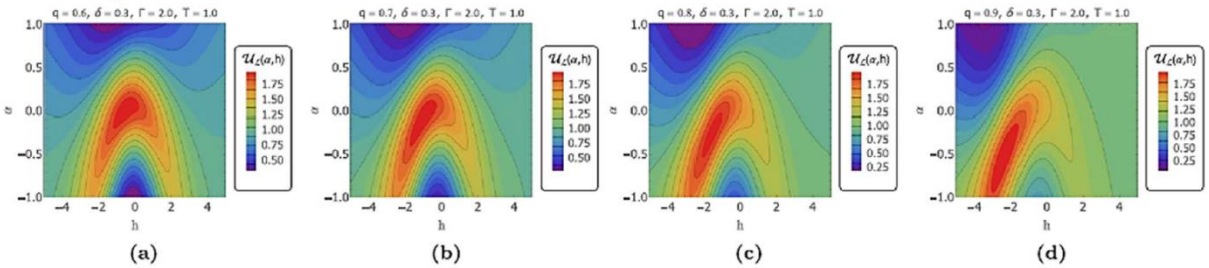
Résumé

Le potentiel des dispositifs quantiques à base de spin pour le traitement de l'information quantique s'élargit constamment. Des nouveaux modèles avec couplages hors-diagonaux permettent d'explorer de nouveaux phénomènes dans la matière condensée. Dans une chaîne de spin XY−Γ à deux qubits en équilibre thermique, nous analysons l'impact de la température, des couplages d'échange hors-diagonaux et du champ magnétique sur les corrélations non-classiques (NCC), la cohérence quantique (QC), la relation d'incertitude entropique (EUR) et le degré de mélange de l'état quantique du système. Les résultats montrent que les NCC connaissent des transitions soudaines tandis que la QC reste stable. Les couplages hors-diagonaux renforcent les NCC et la QC, mais la température et le champ transverse réduisent cet effet. L'incertitude entropique augmente avec la température, atteignant son maximum lorsque le degré de mélange est élevé. Enfin, en utilisant une opération de filtrage appliquée au qubit A, il est possible de réduire l'incertitude de mesure et d'optimiser le transfert d'information entre les qubits,
en ajustant les paramètres du système et la force du filtrage.

Mots clefs: Non-classical correlations, Quantum Jensen-Shannon coherence, Entropic uncertainty, XY
− Γ spin chain, Filetring operation.

Graphical abstract



Reference

[1] A. Ait Chlih et al, Unveiling non-classical correlations, quantum coherence and steering measurement uncertainty in two-qubit XY- **Γ** spin model. OQE 56, 1370 (2024).

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Discrimination of entangled and separable Werner state with a Quantum extreme learning machine

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Abstract

The Quantum Extreme Learning Machine (QELM) has emerged as a powerful tool for various quantum information processing tasks. This presentation presents a QELM protocol for estimating entanglement in Werner states. Werner states are mixed states in two-qubit systems, which are known to exhibit entanglement for certain parameter p ranges. We propose a framework that efficiently estimates the entanglement of Werner states with high accuracy.

The protocol involves generating a sequence of random numbers to define the parameter values p for Werner states. These states are combined with a reservoir state and evolved using a Hamiltonian. We construct a set of observables based on the Bloch basis, which are used to train the system.

We also investigate the robustness of the protocol by introducing noise into the input states and analyzing the system's ability to perform the task under noisy conditions. In addition, we investigate the influence of the magnetic field parameter on the estimation performance.

This presentation aims to highlight the methodology of the protocol, the training process, and the evaluation results. The investigations of the robustness to noise and magnetic field dependence further contribute to our understanding of the protocol's performance characteristics.

Keywords: Quantum extreme learning machine, Werner state, entanglement, estimation

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Non-classical correlations and coherence in a two-dimensional electron gas under the infuence of Rashba spin-orbit coupling

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Résumé

Cette étude explore la dynamique des corrélations quantiques et de la cohérence au sein d'un système de gaz d'électrons bidimensionnel (2DEG), en prenant en compte l'influence du couplage spin-orbite de Rashba (SOC). Nous utilisons des métriques telles que la négativité logarithmique (LN), l'incertitude quantique locale (LQU (U)) et l'entropie relative de cohérence (Cr) pour évaluer spécifiquement ces ressources quantiques entre les spins d'électrons dans des gaz d'électrons non-interagissants. Notre étude examine comment la distance de séparation (R) entre les électrons et l'intensité du SOC de Rashba (α) influencent le comportement des propriétés quantiques dans le système 2DEG. Nous constatons que certaines intensités de SOC de Rashba peuvent réguler efficacement les corrélations et la cohérence quantiques dans ce système. Une observation particulièrement significative est que des indicateurs quantiques optimaux apparaissent lorsque la proximité entre les électrons est minimisée, soulignant l'impact considérable de la distance entre les électrons sur les caractéristiques quantiques. Inversement, à mesure que la séparation des électrons augmente, ces mesures quantiques diminuent. Ainsi, en ajustant le paramètre de Rashba, il est possible d'augmenter la résilience de ces mesures quantiques face à l'augmentation des séparations électroniques, fournissant des informations précieuses pour le contrôle et la manipulation du comportement quantique dans des systèmes similaires de type 2DEG.

Etude des corrélations quantiques dans les systèmes magno-mécaniques

Benrass Noureddine[1], Nabil Habiballah , and Mostafa Nassik

[1]Ibn Zohr University, Faculty of Sciences, Agadir – Maroc

Résumé

Nous étudions la réalisation et le transfert de l'intrication dans un système cavité-magnon constitué de deux cavités positionnées à des endroits différents, chacune contenant un mode de champ micro-onde (MW) et un mode magnon de la sphère de grenat d'yttrium et de fer (YIG).

Entanglement and Bell non-locality versus quantum-memory-assisted entropic uncertainty relation in two 2 level atoms Under the Influence of a Global Environment

Mourad Benzahra and Mostafa Mansour
[2]Laboratory of High Energy Physics and Condensed Matter, Faculty of Sciences Ain Chock, Hassan II University, Casablanca, Morocco – Maroc

Abstract

In this investigation, we delve into the dynamics of entanglement, Bell nonlocality, and the quantum-memory-assisted entropic uncertainty relation (QMA-EUR) within two atoms undergoing a common Markovian dissipative environment. Various quantifiers are employed to evaluate different aspects of the system's quantum characteristics. Specifically, the concurrence and the CHSH-Bell inequality are utilized to gauge entanglement and Bell nonlocality violation, while the QMA-EUR and its lower bound are used to quantify the measurement uncertainty within the considered system. Our findings reveal intriguing distinctions in the behaviors of entanglement, Bell nonlocality, and QMA-EUR. Notably, an increase in the scaled time and the mean number of thermal photons N effectively reduces the degree of entanglement and the violation of the CHSH-Bell inequality, while simultaneously enhancing QMA-EUR. However, we observed that manipulating the parameters defining the initial state of the two-level atom system can enhance both the entanglement and the violation of Bell nonlocality between the two atoms. Remarkably, this enhancement coincides with a reduction in the uncertainty measurement within the system. Additionally, it is noted that these measures employed in the system completely vanish over long times. Our research underscores the importance of precisely adjusting the parameters of the initial system state, prepared in an extended Werner-like state (EWL), to protect quantum resources shared between the two atoms from environmental influences. This adjustment also reveals the crucial relationship between these resources and QMA-EUR in a Markovian system.

Unveiling Thermal Quantum Correlations in a Two-Dimensional Graphene System Under Decoherence Channels

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[1]Laboratory of High Energy Physics and Condensed Matter, Department of Physics, Faculty of Sciences Ain Chock, Hassan II University, Casablanca, Morocco.

Abstract

Two-dimensional graphene systems present considerable advantages for quantum information processing. Electrons within graphene possess not just spin but also additional attributes associated with their specific positions within the lattice and valley index. This study investigates how decoherence channels impact thermal quantum correlations within individual electrons in a two-dimensional graphene system, considering both electron pseudospin and valley index degrees of freedom. Using metrics such as local quantum Fisher information (LQFI), this research evaluates the degree of quantum correlations among these extra degrees of freedom of electrons within the graphene system. The dynamics of the intra-particle quantum correlations in graphene's thermal state is analyzed with respect to factors such as scattering strength, the band structure of graphene, and wavenumber operators. The findings suggest that adjusting the parameters of the graphene system holds promise for enhancing quantum correlations, thereby mitigating the adverse effects of increasing equilibrium temperature. Moreover, the study examines how intra-particle thermal quantum correlations evolve under various decoherence channels, including phase damping (PD), phase flip (PF), and amplitude damping (AD). It is observed that LQFI behaves similarly under AD and PD channels, which diminishes as the decoherence parameter increases. However, distinct behavior is observed when graphene's thermal state undergoes the PF channel, where LQFI displays symmetrical behaviors around the decoherence parameter of p=0.5.

Etude géométrique d'un système à deux spins avec champ magnétique externe

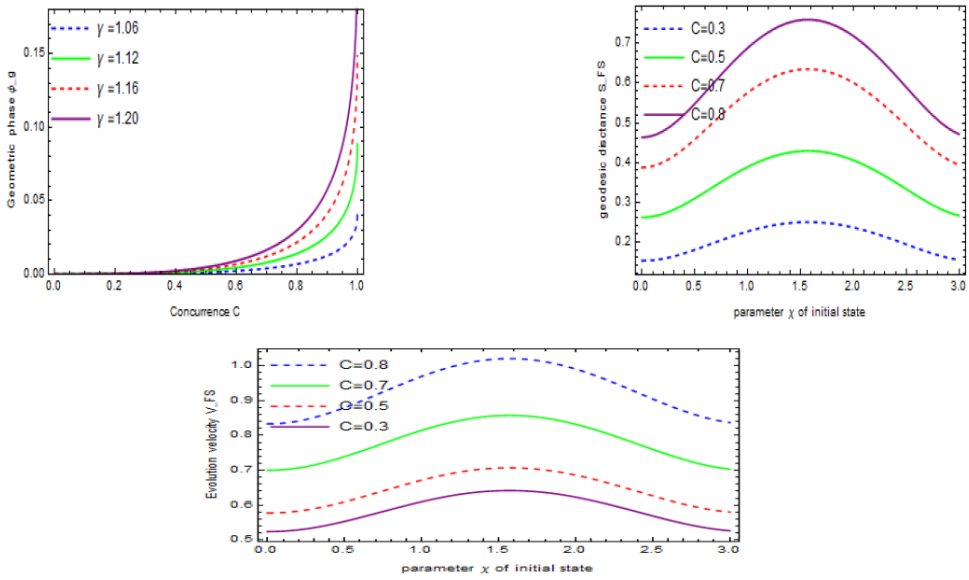
C. Boukacem, B. Amghar, M. EL Falaki

LIMT, Innovation des sciences et Technologie et Modélisation , Faculté des Sciences. Université Chouaib Doukkali El Jadida Département de physique, Faculté des sciences, Université Chouaib Doukkali El Jadida , Maroc

Résumé

La communication est consacrée à présenter la vision de l'approche géométrique et ces outils pour étudier un système quantique tel que la distance géodésique, la phase géométrique la vitesse d'évolution. Ensuite en va appliquer cette approche sur un système à deux spins subit à l'action d'un champ magnétique externe en essayant toujours de visualiser les caractéristiques de ce système, son l'intrication et son évolution dynamique dans une perspective géométrique.

Enfin, on va illustrer l'effet de l'intrication et du champ magnétique externe sur la dynamique de système ainsi sur la phase géométrique.



Mots clé : Variété d'état, phase géométrique, distance géodésique, la métrique de Fubini study.

Corrélations non classiques métrologiques et cohérence quantique dans un système hybride (1/2,1) sous des canaux de décohérence.

Abdessamie Chhieb, Mostafa Mansour [2], and Mohamed Ouchrif[1]
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Résumé

Notre recherche se concentre sur l'interaction entre le bruit thermique et les canaux de décohérence sur la cohérence quantique et les corrélations non classiques dans un modèle hybride de Heisenberg (1/2,1). Ce système hybride intègre l'interaction de Dzyaloshinsky–Moriya (DMI) et fonctionne sous l'influence d'un champ magnétique externe. Nous utilisons l'information quantique locale de Fisher (LQFI) pour l'estimation des corrélations et l'entropie relative de cohérence pour la mesure de la cohérence dans le système étudié. Notre investigation couvre divers paramètres du système hybride, la force du DMI et l'intensité du champ magnétique externe. Nos résultats soulignent que l'élévation de la température compromet les corrélations non classiques ainsi que la cohérence. En revanche, la robustesse du DMI atténue l'impact du bruit thermique sur les corrélations d'information quantique de Fisher et sur l'entropie relative de cohérence dans le système hybride. De plus, nous examinons l'impact des canaux de d´ecohérence - spécifiquement, la d´ecohérence de phase, les canaux de basculement de phase et les canaux de basculement de bit et de trit - sur la cohérence thermique et les corrélations quantiques. L'introduction de divers processus de d´ecohérence dans le système hybride qubit-qutrit conduit `a une compétition avec les fluctuations thermiques, donnant ainsi lieu à des états hors d'équilibre. Nos résultats indiquent qu'à mesure que le paramètre de force de d´ecohérence (p) augmente, `a la fois la LQFI et l'entropie relative de cohérence présentent des comportements similaires dans les canaux de d´ecohérence de phase et de basculement de phase. Ces ressources diminuent progressivement, pour finalement disparaitre complètement `a p=1. Dans le contexte des canaux de basculement de bit et de trit, la cohérence quantique montre des distinctions notables par rapport à ce qui est observé dans les canaux de d´ecohérence de phase et de basculement de phase, révélant que la cohérence peut être préservée si le DMI est fort et si l'intensité du champ magnétique externe est réduite. Ces résultats sont importants car il est essentiel de d'abord comprendre le processus de d´ecohérence, résultant de l'interaction avec l'environnement, puis de trouver des moyens pour entraver cette d´ecohérence afin d'éviter la perte complète des ressources quantiques nécessaires au traitement de l'information quantique.

Thermal quantum correlations of a fermionic system

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Abstract

In this research, we investigate the thermal quantum correlations in a fermionic system modeled using an extended Fermi–Hubbard-like model. We examine the impacts of noisy temperature, local chemical potential, and nearest-neighbor interaction. The Fermi–Hubbard model provides a framework for understanding fermion interactions in a lattice and shows potential for simulating fermionic systems with superconducting circuits in quantum simulation. Using the Jordan–Wigner transformation, we convert the fermionic system into a qubit system, bridging quantum information and particle physics. Thermal entanglement is assessed using concurrence measurement, while thermal quantum correlations are measured through trace distance discord and local quantum uncertainty. Our findings indicate that increasing temperature causes disorder, negatively affecting quantum entanglement and correlations. However, by adjusting the nearest-neighbor interaction strength and local potential, we can mitigate thermal noise effects, enhancing correlations and entanglement. Selecting appropriate parameters can ensure the system's potential for quantum technology development.

Keywords: Thermal quantum correlations, fermionic system, extended Fermi–Hubbard-like model.

Abstract figure:

∗From our recent work: Mohamed Essakhi and Mostafa Mansour, Laser Phys. Lett. 21 105201 (2024).

Controlling transmission and slow/fast light in an optomechanical system with an optical parametric amplifier

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In this paper, we investigate the phenomenon of optomechanically induced transparency (OMIT) in a cavity that has a moving end mirror and is subjected to an external force. Furthermore, we place an optical parametric amplifier (OPA) inside the cavity. We show that the transmission intensity of the probe field and the group delay are enhanced by the parametric gain and phase of the optical parametric amplifier. We also show that this enhancement is influenced by external forces. We believe that these findings could be valuable in the area of quantum information processing.

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Distribution of distance-based quantum resources outside a radiating Schwarzschild black hole

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Abstract

This study aims to investigate the distribution of distance-based quantum resources for fermionic fields in curved Schwarzschild spacetime (SST), as well as for bosonic fields in both flat Minkowski and curved Schwarzschild spacetimes. To achieve this, we will examine the quantum resources between an observer falling into a Schwarzschild black hole (SBH) and their stationary partner, who shares a Gisin state. Additionally, we will explore the quantum resources that arise when two uniformly accelerated detectors interact with bosonic fields in the Minkowski vacuum. Furthermore, we will investigate the interactions between these detectors and bosonic fields in the Hartle-Hawking and Boulware vacuums outside the SBH. At an infinite Hawking temperature, the quantum resources for the fermionic fields degrade; the rate of degradation is dependent on the distance between the observer and the event horizon (EH), the fermionic frequency mode, and the Gisin state parameters. In the case of the bosonic fields, our results show that entanglement decreases monotonically, either towards zero or a constant value. Moreover, with increasing Unruh temperature, coherence and discord undergo sudden death followed by a sudden birth, and entanglement cannot be revived for a given initial state. Based on our findings, it appears that the Fermi-Dirac and Bose-Einstein statistics represent the primary differences in quantum resource distribution between the fermionic and bosonic cases. These findings may be essential for enhancing our understanding of the distribution of quantum resources in relativistic frameworks.

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L'étude des dynamiques des corrélations quantiques sous l'influence combinée des bruits d'amplitude et de phase

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Abstract

We study the dynamics of quantum correlations in an anisotropic XYZ Heisenberg chain under the combined influence of amplitude and phase damping noise. Our model incorporates Dzyaloshinskii-Moriya (DM) and KSEA interactions along the z-axis, along with anisotropic Heisenberg interactions. We analyze the eigenvalues and eigenstates of the system to understand the effect of the noise. Using Kraus operators, we model the time evolution of the initial density matrix. The results show how the purity and Bell non-locality properties evolve under these noise conditions. We reveal complex dynamics that depend on the coupling parameters and noise rates. This study provides new insights into the combined effects of amplitude and phase noise on anisotropic quantum systems, with implications for the development of quantum technologies resilient to environmental noise.

Coherence versus quantum-memory-assisted entropic uncertainty relation of double quantum dots with Rashba spin-orbit interaction

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Abstract

Gaining insight into nanostructure devices represents a crucial step in unlocking their full quantum potential. Solid-state quantum dots provide a practical and scalable foundation for implementing qubits, which are essential for quantum information processing. In this context, we introduce a model involving a pair of qubits within a double quantum dot configuration. We investigate its quantum coherence and the quantum-memory-assisted entropic uncertainty relation (QMA-EUR), considering the influence of the temperature and Rashba spin-orbit coupling. Our findings reveal a monotonic increase in QMA-EUR with rising temperatures, while Jensen-Shannon coherence consistently decreases as temperature increases. Furthemore, fine-tuning the Rashba coupling can enhance the system's coherence and reduce measurement uncertainty. We show that obtaining higher measurement precision is achievable when the two-qubit system demonstrates higher levels of coherence.

Quantum simulation

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Abstract

In this poster presentation, I will describe the digital, analog, and hybrid (digital-analog) paradigms of quantum computing. Additionally, I will discuss the potential applications of the quantum Rabi model, with a particular focus on implementing deep strong coupling use cases using current quantum computers in circuit quantum electrodynamics (cQED).

The quantification of correlations in three levels laser systems

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Abstract

The utilization of three-level systems within doubly resonant cavities connected to a shared two-mode thermal reservoir presents a wide array of important applications in quantum technologies. In the realm of quantum information processing, these systems enable the realization of quantum gates and function as repositories for quantum information, ensuring the coherent manipulation and retention of quantum data. In quantum communication, these systems are crucial for producing entangled states vital for processes like quantum teleportation and for extending communication ranges via quantum repeaters. Furthermore, they play a key role in quantum thermodynamics by facilitating the investigation of quantum heat engines and thermal entanglement, providing insights into the significance of quantum coherence and correlations. Moreover, in the field of cavity quantum electrodynamics (QED), these systems permit the exploration of strong coupling phenomena such as vacuum Rabi splitting and photon blockade, which are indispensable for generating single-photon sources and conducting quantum non-demolition measurements. progression of quantum information science and technology.

InAs three quantum dots as working substance for quantum heat engines

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Abstract

Heat engines are considered a valuable resource for the modern society. The development of these systems leads to the production of heat engines with high efficiency despite their small size, called quantum heat engines. Among these, the quantum Otto cycle which is considered a fundamental thermodynamic cycle in classical heat engines, has also found applications in the realm of quantum heat engines. In this paper, we consider three InAs quantum dots as a working substance, which allows the engine to operate at very small scales, in the presence of an electric eld, and the Förster mechanism, which describes the transfer of energy between quantum dots and thus affects the engine's behavior. In this regard, we study the behavior of the work performed by the engine and the entanglement in the system as the Förster parameter is varied. We found a significant link between the engine's work performance, the system's entanglement, and the Förster interaction. At a critical Förster interaction value, which depends on the excitons frequencies, we observe a sharp infection in work output. This transition coincides with the system reaching maximum entanglement after a separable state.

2) Physique des Particules, Physique Médicale, Physique Nucléaire et Astrophysique

Three-body semi-leptonic decay of a charged kaon assisted by a laser field

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Abstract

We study the three-body semi-leptonic decay of a charged kaon (K) in the presence of an intense laser field. This research explores the effects of laser-particle interactions on decay processes, highlighting changes in decay rates due to the laser field. We use a theoretical approach based on perturbation theory in the first born approximation to model these interactions and calculate the transition amplitude. The results show that the laser field can significantly influence kaon decay, opening up new perspectives for the study of fundamental interactions under extreme conditions.

Revisiting theoretical constraints in the N2HDM

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Abstract

We investigate how the Next-Two-Higgs Doublet Model extension (N2HDM) should look if we are to address the naturalness problem using dimensional regularization. Our calculations of the overall quadratic divergences have been performed with full consistency with the latest data from the Large Hadron Collider (LHC) concerning the observed 125 GeV Higgs boson, alongside precision electroweak data tests and lower mass limits on charged Higgs boson. It is shown that the quadratically divergent quantum corrections δi (i=1,2,3) for the three CP-even Higgs bosons are controllably small, though hidden fine-tuning might still be required. This significantly impacts the model parameter space, Higgs spectrum mass and notably the singlet-doublet admixture.

Keywords: Particle Physics, Beyond Standard Model, Higgs Physics, Naturalness, LHC (CERN).

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On Stability Behaviors of 5D M-theory Black Objects on three-parameter Calabi Yau Geometry

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Abstract

In this work, we reconsider the study of 5D black branes in M-theory compactifications by means of N=2 supergravity formalism. Precisely, we provide a model relaying on a three parameter Calabi{Yau (CY) manifold in the projective space factorization, referred to as economical model. First, we investigate the stability of 5D BPS and non-BPS black holes obtained from wrapped M2-branes on nonholomorphic two-cycles in such a CY manifold. Then, we approach the stability of 5D black strings derived from wrapped M5-branes on nonholomorphic four-cycles. Among others, we find various stable and unstable black brane solutions depending on the charge regions of the involved moduli space.

Enhancing Quality Assurance in External Radiation Therapy: A Study on the Use of EPID ASi1200 and ArcCHECK® Phantom in VMAT Plans

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Abstract

Background: With the increasing use of volumetric modulated arc therapy (VMAT) treatment techniques and the complexity of the associated treatment plans, there is a growing need for robust patient quality assurance protocols. This study aims to verify VMAT plans using ArcCHECK® and the ASi1200 EPID (electronic portal imaging device), followed by a comparative analysis.

Methods and Materials: A total of 73 VMAT treatment plans for brain, abdomen, chest, pelvis, and head and neck cancers, calculated using the Eclipse treatment planning system (TPS) for TrueBeam STx linear accelerator photon beams with an energy of 6 MV, were evaluated. The TPS-calculated doses were compared to measured ones using an ArcCHECK® phantom and the ASi1200 EPID. A 2D Gamma index test with a 3%/3 mm criterion and a 10% threshold was conducted to perform the comparisons.

Results: Both the EPID ASi1200 and the ArcCHECK® phantom demonstrated the capability to conduct VMAT plan verification. However, a comparative analysis of gamma index results revealed discrepancies in the quality assessment of the evaluated plans between the two devices.

Conclusion: Relying solely on a single device may not ensure patient-specific quality assurance for complex VMAT treatment plans. To protect patients from potential errors caused by machines or humans, it is recommended to utilize both the EPID ASi1200 and the ArcCHECK® phantom. This combination allows for a comprehensive evaluation of the quality of complex VMAT plans across different types of cancer.

Keywords: Quality Assurance, Pre-treatment Verification, VMAT, Portal Dosimetry, EPID, ArcCHECK®

Etude de la diffusion électron-nucléon sous l'influence d'un champ laser monochromatique

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Résumé

Ce travail nous a permis de présenter l'étudier du processus de diffusion électron nucléon, où ce dernier est considéré sans spin et avec une structure sphérique, en absence et en présence d'une onde électromagnétique monochromatique polarisée circulairement. À l'aide du formalisme de Dirac Volkov, nous avons donné l'expression final de la section efficace différentielle (SED). Ce travail est structuré de façon de donner deux comparaisons, premièrement entre (SED) en absence et en présence du champ laser et deuxièmement entre les deux diffusions électron proton et électron neutron. Les résultats de discussion de l'effet du champ laser sur la (SED) et le facteur de forme électrique ont été abordé dans ce travail pour les deux cas de diffusion. Nous avons constaté que les (SED) diminuent en appliquant le champ laser, et le facteur de forme diminue en augmentant l'´énergie incidente de l'électron, alors qu'il reste intact pour des intensités électriques variants jusqu'à 10^8 V/cm.

Search for Magnetic Monopoles Using the Complete ANTARES Neutrino Telescope Dataset

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Abstract

This study presents a novel investigation into magnetic monopoles using data collected over a 14-year period (2008{2022) by the ANTARES neutrino telescope. Upper limits on the ux of magnetic monopoles are established for velocities both above and below the Cherenkov threshold, The interaction of magnetic monopoles with matter was modeled according to Kasama, Yang, and Goldhaber cross-section. No events consistent with the passage of relativistic magnetic monopoles were detected, enabling the setting of an upper ux limit for ultra-relativistic magnetic monopoles at approximately $3.2\times10^{-18}cm^{-2}s^{-1}sr^{-1}$.

Keywords: ANTARES telescope, Magnetic Monopoles, water-cherenkov detector

Evaluating Time-of-Flight Particle Identification Performance Using ePIC Software at the Electron-Ion Collider

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Abstract

The Electron-Ion Collider (EIC) represents a groundbreaking opportunity to explore the fundamental structure of nuclear matter with unprecedented precision. A critical component of its success is the ability to achieve robust particle identification (PID) across a wide kinematic range. The Time-of-Flight (TOF) detector, in combination with the EIC Particle Identification Consortium (ePIC) software framework, plays a pivotal role in meeting this challenge by providing precise velocity measurements essential for distinguishing between hadron species.

This work presents a comprehensive evaluation of the TOF PID performance utilizing the ePIC simulation and reconstruction toolkit. We assess the system's capability to identify particles based on timing resolutions under varying detector configurations, beam energies, and collision environments. Key metrics, such as PID efficiency, purity, and resolution, are analyzed to quantify the TOF system's robustness. The interplay between TOF performance and other sub-detectors is also explored to highlight the integrated capabilities of the ePIC framework.

Our findings demonstrate the TOF detector's ability to meet the demanding PID requirements of the EIC physics program, enabling high-fidelity separation of pions, kaons, and protons up to several GeV/c. The implications of these results for optimizing detector design and advancing simulation methodologies are discussed. This study provides essential insights that will shape the EIC's detector optimization strategies, ensuring the delivery of transformative science in the study of quantum chromodynamics.

This contribution offers a pivotal assessment of the synergy between TOF hardware and state-of-the-art software tools, laying the foundation for precise particle identification in the era of the EIC.

Decelerating quantum decay processes via strong electromagnetic fields

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Abstract

The rapid development of laser technology has paved the way for the use of laser sources to study relativistic processes in the fields of quantum electrodynamics, atomic physics and high-energy physics. In this context, the main purpose of this talk is to advance our understanding of the ultrafast physical processes that occur in the presence of a laser field. It therefore belongs to the research field called strong-field physics, which is the general research area of laser-matter interaction. Specifically, we focus on a new theoretical study, in the framework of electroweak theory, of the decay processes of the W and Z bosons in the presence of a circularly polarized laser field. This study revives the controversial debate that has arisen over the last two decades about the possibility that the electromagnetic field affects the lifetime or decay rate of an unstable particle.

Effet du champ électromagntique sur la désintgration du boson de Higgs charge dans le modèle deux doublets de Higgs de type II

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Abstract

In this paper, we investigate the charged Higgs boson decay in the context of the type-II two-Higgs-doublet model in the presence of a circularly polarized electromagnetic field of laser radiation.

The calculations are performed by adopting the Furry picture approach of nonperturbative interactions with the external electromagnetic field. Using the method of exact solutions for charged particles states in the presence of a circularly polarized electromagnetic wave field and evaluating the S-matrix elements, an exact analytic expression is derived for the decay width of leptonic, hadronic and bosonic decay modes. The branching ratios of different decay modes with multiple photon emission and absorption from the laser beam are analyzed and found to be dramatically modified in the region of superstrong fields. The dependencies of the decay width on the laser field strength and frequency are also examined. The results obtained may be interesting for future experimental and theoretical investigations.

Laser-assisted scattering and decay processes in standard model of particle physics

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Abstract

Advanced laser facilities provide very intense light with very short pulses, making it possible to produce new phenomena in the laboratory and reproduce those already observed in the vicinity of high- radiation stars in the universe. As a result, a considerable amount of theoretical research is being carried out, particularly into the scattering processes of particles dressed by these extreme light sources. In this context, the aim of this work is to study the production and decay processes of the standard model and beyond in the presence of a strong electromagnetic field created by a laser instrument. The major investigation of the research presented in this work is the study of the scattering processes in the relativistic laser-assisted collision e^+e^- such as the associated production of the Standard Model Higgs boson and Z^0, and laser-induced decay processes such as the decay of the proton into neutron, positron and electron neutrino.

Keywords: Standard model and beyond, Electroweak interaction, Laser-assisted processes, e^+e collider.

Performance of the missing transverse momentum triggers for the ATLAS detector

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Abstract

The Missing transverse energy (MET) trigger is a crucial part of the ATLAS detector at the Large Hadron Collider (LHC), identifying events with significant missing transverse momentum for further analysis. The trigger system consists of two levels: Level-1 Trigger (L1), a hardware-based system, and High-Level Trigger (HLT), a software-based system. The MET trigger relies on data from calorimeters, which measure the energy deposited by particles in the transverse plane. The ATLAS trigger system has been significantly upgraded. The performance of Missing Transverse Energy (MET) triggers is a crucial aspect of ensuring the efficiency and accuracy of data collection. for that we will study the performance of the MET trigger by using data collected during 2023 & 2024. Performance in terms of efficiency, trigger stability, background rejection, etc. studied as a function of several quantities, including run conditions and pile-up.

MIRD Human phantom external exposure scenarios to ionizing radiation: Modeling with Geant4

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Abstract

From a radiation protection perspectives, the availability of a database collecting dose factors for different types of exposure to radioactive sources is fundamental for the prediction and prevention against the harmful effects of ionizing radiation. In this context, the use of Monte Carlo codes in general and Geant4 in particular, whose basic principle is based on the random choice of the interaction of radiation with matter, seems at first sight, inconsistent with the rigor and precision asked for during metrology measurements. Nevertheless, the considerable benefits that they are supposed to bring, in particular the very comprehensive consideration of the elementary physical phenomena involved in each interaction and the possibility of a very precise description of the geometry and chemical composition of the detector or dosimeter in its real environment, allow us to expect a precise and targeted determination of the physical quantities required, in particularly those items that are inaccessible to the experiment.In this study, we introduce a scenario of external exposure to ionizing radiation simulated by Geant4 (Monte Carlo code C++ developed at CERN in the form of a data library and tools that the user can assemble according to his specific needs), where a person (MIRD human phantom provided by Geant4 toolkit) will be exposed to different configurations of radioactive sources that may actually occur as mentioned in reference [1] [2]. The objective is to evaluate the absorbed dose as well as the equivalent dose of each configuration adopted in this scenario.

Keywords Absorbed dose · Equivalent dose · Geant4 code · Radiation protection.

Gammatone Cepstral Coefficients with Empirical Mode Decomposition (EMD): A Hybrid Method for Diagnosing Cardiovascular Disease

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Abstract

Automatic diagnosis has become essential in modern healthcare systems, providing rapid solutions for early disease detection. Among biomedical signals, the phonocardiogram (PCG) stands out as a crucial non-invasive tool for assessing cardiovascular conditions. However, extracting and analyzing meaningful features from PCG signals remains challenging due to their complexity and noise.

Recent advances in signal processing, such as cepstral analysis and multiresolution techniques, have significantly improved the reliability of PCG-based diagnosis by capturing temporal and spectral details. This study proposes a hybrid model combining two complementary approaches: Empirical Mode Decomposition (EMD) to extract intrinsic components and gammatone cepstral coefficients to model spectral properties accurately.

Using cross-validation and ensemble learning, this method achieved an accuracy exceeding **85%**, demonstrating its effectiveness. This multidimensional approach enhances the robustness and precision of diagnostic models, addressing the complex challenges of cardiovascular disease diagnostics in modern healthcare.

Keywords: Automatic diagnosis, Phonocardiogram (PCG), Cardiovascular diseases, Signal processing, Empirical Mode Decomposition (EMD), Gammatone cepstral coefficients, Ensemble learning, Multiresolution analysis, Cross-validation

Evaluation of Alpha and Lithium-7 Energy Release in BNCT: A Geant4 Simulation Approach

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Abstract

Boron Neutron Capture Therapy (BNCT) represents a promising approach for treating aggressive cancers, particularly brain tumors. This study employs advanced Monte Carlo simulations using Geant4 to explore the microdosimetry of BNCT at the cellular level, focusing on energy deposition patterns of alpha particles and lithium-7 ions resulting from the 10B(n,α)7Li reaction. We compared various physics lists (G4QGSP_BIC_HP, Geant4-DNA, G4QGSP_BIC) and water models (H2O, G4_WATER) in a detailed single-cell model and multi cell model. Results demonstrate overall consistency among physics lists, with subtle yet significant differences in energy deposition predictions. Alpha particles deposit the majority of their energy within close proximity to their origin, primarily in the cell nucleus, while lithium ions exhibit a more diffuse deposition pattern. Cellular compartment analysis reveals that the nucleus consistently receives the highest energy deposition, followed by the cytoplasm and cell membrane. These findings provide crucial insights for optimizing BNCT protocols, highlighting the importance of precise boron compound delivery to maximize tumor cell damage. The study also underscores the need for standardization in simulation protocols to ensure comparability across different studies. Future perspectives include extending simulations to multicellular systems, incorporating more complex cellular geometries, and validating results against experimental data, paving the way for more effective and personalized BNCT treatments.

Analyse Comparative de la Dosimétrie entre la RC3D et la RCMI pour les Cancers Mammaires Gauches

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Résumé

La radiothérapie des cancers du sein entraine souvent une toxicité pour les organes à risque comme les poumons et le cœur. Cette étude compare la dosimétrie de la RC3D et de la RCMI chez 20 patientes atteintes d'un cancer du sein gauche. Les résultats montrent que la RCMI améliore la distribution de dose dans les volumes cibles et réduit la toxicité pour les organes à risque par rapport à la RC3D. La RCMI s'avère donc plus efficace pour assurer une couverture adéquate des volumes cibles tout en minimisant les effets indésirables.

Measurement of light-by-light scattering with the ATLAS detector at the Large Hadron Collider

Ghizlane Ez-zobayr

IAP-UM6P

Abstract

Light-by-light (LbyL) scattering, is a quantum-mechanical process described by quantum electrodynamics (QED). The first evidence of this phenomenon was published by the ATLAS Collaboration in 2017. We are currently working on a new measurement of light-by-light scattering in lead-lead (Pb+Pb) collisions using Run 3 data, recorded by the ATLAS experiment at the Large Hadron Collider (LHC). Our aim is to improve upon previous measurements by reducing uncertainties and searching for new physics. Our results will provide a more precise understanding of light-by-light scattering, contribute to testing the predictions of QED, and probe new physics.

Our contribution consists of measuring the fiducial cross-section and four differential distributions of the scattering process. To achieve this, we employ statistical techniques such as bin-by-bin unfolding and iterative Bayesian unfolding. These methods allow us to correct the detector effects and extract the true distributions of the physical quantities of interest.

In this presentation we will showcase the concept of light-by-light scattering and discuss the statistical techniques employed in its measurement.

Swampland Statistics for Black Holes

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Abstract

In this work, we approach certain black hole issues, including remnants, by providing a statistical description based on the weak gravity conjecture in the swampland program. Inspired by the Pauli exclusion principle in the context of the Fermi sphere, we derive an inequality which can be exploited to verify the instability manifestation of the black holes via a characteristic function. For several species, we show that this function is in agreement with the weak gravity swampland conjecture. Then, we deal with the cutoff issue as an interval estimation problem by putting an upper bound on the black hole mass scale matching with certain results reported in the literature. Using the developed formalism for the proposed instability scenarios, we provide a suppression mechanism for the remnant production rate. Furthermore, we reconsider the stability study of the Reissner-Nordstrom black holes. Among others, we show that the proposed instabilities prohibit naked singularity behaviors In this work, we approach certain black hole issues, including remnants, by providing a statistical description based on the weak gravity conjecture in the swampland program. Inspired by the Pauli exclusion principle in the context of the Fermi sphere, we derive an inequality that can be exploited to verify the instability manifestation of the black holes via a characteristic function. For several species, we show that this function is in agreement with the weak gravity swampland conjecture. Then, we deal with the cutoff issue as an interval estimation problem by putting an upper bound on the black hole mass scale matching with certain results reported in the literature. Using the developed formalism for the proposed instability scenarios, we provide a suppression mechanism to the remnant production rate. Furthermore, we reconsider the stability study of the Reissner-Nordstrom black holes. Among others, we show that the proposed instabilities prohibit naked singularity behaviors.

Recherche de résonances dimuons de faible masse avec le détecteur ATLAS avec des données de collision 140 fb-1 pp à √s = 13 Tev

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Résumé

Recherche d'une nouvelle résonance dans les événements caractérisés par un état final de dimuon dans la région de masse inférieure à celle du pôle du boson Z en utilisant les données complètes d'ATLAS Run 2 140 fb-1. La forme du signal est obtenue par la convolution d'une fonction Breit-Wigner et d'une fonction Crystall-Ball à double face. La régression du processus gaussien s'avère capable d'ajuster la forme de masse complexe du système $\mu\mu$ $S + B$. L'ajustement basé sur la technique de régression GP est introduit pour un ajustement de masse afin d'extraire les signaux. Des tests de linéarité comprenant une étude des signaux parasites et des études d'injection de signaux sont effectués pour valider l'approche de régression GP pour la modélisation de fond.

Search for Charged Higgs Bosons in Bosonic Decays with Diphoton Final States with the ATLAS Detector

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Abstract

This study searches for the production of a charged Higgs boson in association with a top and a bottom quark ($pp \rightarrow tbH^{\pm}$) using the full Run-2 ATLAS dataset. The analysis focuses on the novel decay channel $H^{\pm} \rightarrow W^{\pm}A$, with $A \rightarrow yy$, in 0-lepton and 1-lepton final states. Motivated by Two-Higgs-Doublet Models (2HDM), this search explores benchmark scenarios with varying mA and $mH^{\pm}$, leveraging the clean diphoton signature to probe new physics.

Exploring Nuclear Structure in the Isotopic Chain of Iodine: Insights into Transitional Nuclei Around A≈120

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Abstract

The isotopic chain of iodine nuclei 113,115,117I in the mass region A≈120 exhibits a rich interplay of single-particle and collective excitations, making it a valuable subject for nuclear structure investigations. In this work, we employ the Nilsson model, the BCS method, and the TammDancoff Approximation (TDA) to calculate the low-energy states of these nuclei. The model includes key interactions such as quadrupole-quadrupole coupling, pairing interactions, and recoil effects, complemented by rotational motion corrections. To refine our predictions, we incorporate the Quasiparticle-Phonon plus Rotor Model (QPRM), enabling a detailed study of vibrational and rotational excitations. Preliminary results highlight the emergence of specific band structures and transition probabilities that are consistent with experimental data, while offering new insights into the underlying nuclear dynamics. These findings provide a phenomenological framework for understanding the evolution of nuclear shapes and excitation mechanisms in this transitional region.

Keywords: Nuclear structure Quantum mechanics Nilsson model QPRM model.

Constrained Deflection Angle and Shadows of Rotating Black Holes in Einstein-Maxwell-scalar Theory

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Abstract

In this talk, we investigate the constrained optical properties of rotating black holes in the Einstein-Maxwell-scalar gravity theory with the presence of a stringy parameter. Using the Hamilton-Jacobi algorithm, we derive certain shadow geometries, corroborated by observational data when appropriate constraints on the coupling parameter are imposed. For these constrained regions, we compute and analyze the deflection angle of light rays near such black holes

3) Physique des Matériaux

Investigation of electronic, thermodynamic, and optical properties of LiTi2O4 cathode material for Li-ion battery: An Ab Initio calculations

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Abstract

In this research, we have conducted an in-depth investigation into the structural, electronic characteristics, and thermodynamic properties of the LiTi2O4 compound using first-principles calculations grounded in density functional theory with the generalized gradient approximation. Our findings reveal that the LiTi2O4 compound possesses a calculated lattice constant of 8.407 Å. Furthermore, we have derived critical battery-related properties, including an average voltage of 1.53V versus Li/Li + and an energy density of 245 Wh/kg. To deepen our understanding of LiTi2O4 , we have explored its thermodynamic properties employing the quasi-harmonic Debye model. These properties encompass the Debye temperature, volume variation, compressibility modulus, specific capacity, and thermal capacity. Importantly, we have observed that the Debye stiffness of LiTi2O4 increases with rising pressure. Moreover, we have conducted measurements to assess various optical properties of the LiTi2O4 compound. These properties include the absorption coefficient, photoconductivity, and reflectivity.

Keywords: LiTi2O4 ; Li-Battery; DFT; Average voltage; Absorption coefficient, photoconductivity, and reflectivity.

Magnetic properties of six-legged spin-1/2 nanotube in presence of a longitudinal applied field

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Abstract

Hexagonal spin nanotube is studied using the Effective Field Theory with correlations (EFT) and the differential operator technique (DOT). Each spin is connected to the nearest-neighbors through exchange couplings both along the chains ($J_{//}$) and adjacent chains ($J_{\perp}$). The effects of the exchange, the single-ion anisotropy and the magnetic field on the phase diagram and the magnetic properties have been examined. It is shown that the longitudinal and transverse exchange parameters have strong effect on the shape of the phase diagram. Some original behaviors have been emerged. In particular, when the two exchange parameters are opposite, strong frustrations occur, a typical magnetization plateaus and jumps appear.

Keywords:

Hexagonal spin nanotube, Effective Field Theory, exchange couplings, magnetic properties, magnetic

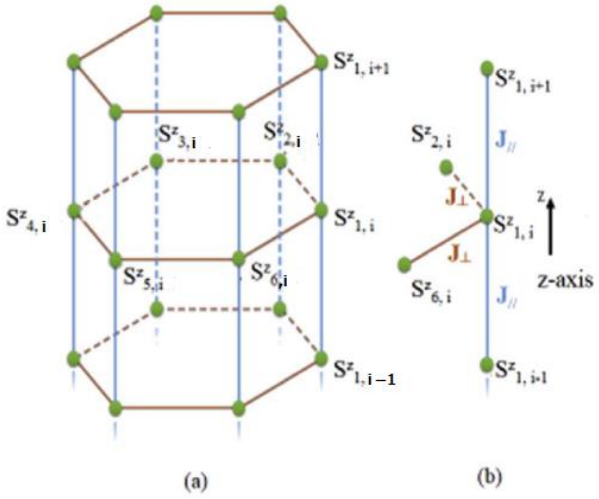

Fig. 1. Schematic structure of the hexagonal spin ½ tube (a). The longitudinal (J//) and the transverse (J⊥) exchange couplings are

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Investigating the physical characteristics of cubic perovskite oxides (SrSiO3) theoretically

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Abstract

Various physical properties (electronic and optical) of cubic perovskite oxides $SrSiO_3$ are investigated by using the density functional theory (DFT) within Wien2K code. This code is based on different approximations such as generalized gradient approximation GGA, PBEsol, LDA, WC and the modified Becke–Johnson exchange potentials (mBJ, nmBJ and unmBJ). Structural properties and the optimization have been calculated using PBEsol functional which showed a significant results that are in good agreement with the experimental ones. The results for physical properties such as electronic and optical are analyzed in detail by using the nmBJ approximation. The obtained results present an opening gap for $SrSiO_3$ An average of transmittance which is about 94% to 97% was observed in the range of visible light.

Keywords : DFT, Wien2k, Perovskite, NmBJ, Electronic and Optic.

Theoretical Investigation of New Semiconducting MXenes for Water Splitting via Visible-Light Photocatalysis

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Abstract

In this paper, we investigates the structural, electronic, optical, and photocatalytic properties of the Sc 2 XT 2 MXene system (X = C or N ; T = Cl or H) to expand the potential of semiconducting MXenes for photocatalytic applications. The study employs density functional theory (DFT)-based theoretical calculations to explain the fundamental properties of these two-dimensional materials and assess their suitability for photocatalytic processes. Thermal and dynamic stabilities of all investigated mono- layers were corroborated through ab initio molecular dynamics (AIMD) simulations and phonon dispersion calculations. These computational methods provided robust evidence for the structural stability of the Sc 2 XT 2 MXene materials under various thermal con-ditions and vibrational modes. Electronic band structure calculations were performed utilizing both PBE-GGA and HSE06 exchange-correlation functionals. The computed band gap energies exhibited significant variations depending on the composition of the X element and the nature of the surface termination

Keywords: DFT, Mxenes, AIMD, monolayer, stability, optoelectronic.

Magnetic properties and phase diagrams of 2D mixed Ising model: A Monte Carlo study

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Abstract

In this study, we explore the ground state phase diagrams and magnetic properties of a two-dimensional ferrimagnet system characterized by alternating spins of values = 3/2, and S = 3 on a square lattice, using Monte Carlo simulation (MCS). We investigate the effect of different exchange interactions, crystal field and external magnetic field on magnetic properties, susceptibility, critical and compensation temperatures, and hysteresis loops. We analyze the phase diagrams, specifically , and , across various values of the exchange interactions, crystal field and the external magnetic field. We found that the compensation temperature starts to evolve significantly for > 0.2 and for > -3 of the spin-3 assembly. On the other hand, the effect of exchange coupling J3 and the crystal field do not exhibit threshold values, resulting in a constant compensation temperature. We observe the N-, Qand P-type compensation behaviors in the system. Additionally, our results indicate that the phase diagrams demonstrate only a second-order phase transition to a paramagnetic phase, with no evidence of a tricritical point.

Optical and Thermo-Plasmonic Properties of Gold Nanoparticles Near a Graphene Structure

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Abstract

The insertion of gold nanoparticles (AuNPs) into graphene (Gr) allows for the creation of hybrid materials with special properties, paving the way for numerous novel applications in a variety of scientific and technological domains. However, research in this sector is still being conducted to improve the preparation, stability, and performance of these plasmonic composites. The interaction of Gr with AuNPs and its effect on the latter's surface plasmon resonance (SPR) is critical in these applications. In this work, we used the finite element method (FEM) to study the plasmonic properties and enhancement nearfield effect in the AuNPs-Gr nanocomposites with different arrangements. The SPR properties and field enhancement capability of AuNPs-Gr nanohybrids are investigated for different arrangements configurations. In particular, the position and amplitude of the SPR peak, as well as the amplitude of the field enhancement coefficient, can be adjusted depending on how the AuNPs are connected to the Gr sheets and the orientation of the system with respect to the direction of the incident field. According to our results, the integration of AuNPs with Gr is an approach often sought for the creation of hybrid materials with desirable properties for optical, photoelectric, photocatalytic and thermoplasmonic applications.

Enhancing Solar Cell Efficiency: A Comparative Study of Lead-Free Double Halide Perovskites Rb_2XAsBr_6 (X= Cu,Tl) using DFT and SLME Methods

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Abstract

Recent advancements and developments in photovoltaic materials have made significant progress owing to the search for efficient and sustainable energy sources. Although lead halide perovskites have demonstrated impressive performance in solar cell applications, they face challenges such as environmental instability and lead toxicity. This study investigates several physical properties of two lead-free double halide perovskites, $Rb_2CuAsBr_6$ and $Rb_2TlAsBr_6$, and evaluates their potential for solar cell applications using density functional theory (DFT) within the Wien2k code and spectroscopic limited maximum efficiency (SLME) approach. The negative formation energy and Born criteria confirm the structural stability of both perovskites in the ideal cubic structure. Optoelectronic analyses reveal that $Rb_2TlAsBr_6$, with a direct band gap of 1.51 eV, exhibits better photovoltaic characteristics compared to $Rb_2CuAsBr_6$, which has an indirect band gap of 0.60 eV. Additionally, the SLME analysis shows that $Rb_2TlAsBr_6$ achieves a higher SLME of approximately 31.4%, compared to $Rb_2CuAsBr_6$ which has an SLME of 7.44%. Moreover, the calculated thermoelectric properties show that $Rb_2TlAsBr_6$ exhibits enhanced thermoelectric performance compared to $Rb_2CuAsBr_6$. These findings highlight the potential of lead-free perovskites, particularly $Rb_2TlAsBr_6$, for next generation solar cell applications.

Keywords: DFT, Wien2k, Rb_2XAsBr_6 (X = Cu, Tl), effective masses and Perovskite solar cells.

Reference [1] Fatihi, H., et al. "Enhancing Solar Cell Efficiency: A Comparative Study of Lead-Free Double Halide Perovskites $Rb_2CuAsBr_6$ and $Rb_2TlAsBr_6$ using DFT and SLME Methods." *Journal of Inorganic and Organometallic Polymers and Materials* (2024): 1-14.

Studying the physical properties of cubic perovskite oxides Based on DFT

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Abstract

Divers propriétés physiques (électroniques et optiques) d'oxyde de pérovskite cubique SrGeO3 ont été étudiées en utilisant la théorie de la fonctionnelle de la densité (DFT) au sein du code Wien2K. Ce code est basé sur différentes approximations telles que l'approximation du gradient généralisé GGA, PBEsol, LDA, WC et les potentiels d'échange modifiés de Becke-Johnson (mBJ, nmBJ et unmBJ). Les propriétés structurales et l'optimisation ont été calculées en utilisant la fonctionnelle PBEsol, qui a montré des résultats significatifs en bon accord avec les résultats expérimentaux. Les résultats pour les propriétés physiques telles que les propriétés électroniques et optiques sont analysés en détail en utilisant l'approximation nmBJ. Les résultats obtenus présentent une ouverture de bande interdite pour SrGeO3. Une moyenne de transmittance d'environ 94% à 97% a été observée dans la gamme de la lumière visible.

Keywords : DFT, Wien2k, Perovskite, NmBJ, Electronic and Optic.

Study of Oxygen Matter Distribution using Glauber Model

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Abstract

The distribution of matter in neutron-rich oxygen isotopes ($^{19-24}$O) is investigated using reaction cross-section measurements with 12C and 28Si targets, applying the Coulomb-modified Glauber model (CMGM). The study examines how reaction cross-sections vary with energy over a broad range (33–980 MeV/nucleon), achieving strong consistency with experimental data when employing a two-parameter Fermi (2pF) density distribution. This approach refines the size parameter (r_{2pF}) and the diffusivity parameter a_{2pF}) through a chi-square optimization method. These optimized parameters allow the determination of matter density distributions and root mean square (rms) radii for $^{19-24}$O isotopes, shedding light on their nuclear structure.

Keywords: Nuclear structure, density distribution, reaction cross section, Glauber model

Reference

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Characterizing scintillation properties using DFT method

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Abstract

Elpasolite materials have attracted significant attention in radiation detection research due to their promising scintillation characteristics. In this study, we utilize Density Functional Theory (DFT) to delve into the atomic-level behavior of elpasolite scintillators. Employing computational simulations, our goal is to unravel the electronic structure, optical attributes, and dynamics of excited states within these materials. Our results yield crucial insights into the fundamental mechanisms that drive the scintillation phenomena in elpasolites, thereby enhancing our comprehension of their performance for diverse applications in radiation detection and imaging technologies.

Structural and microstructural properties of $Ba_{0.54}Ca_{0.46}Fe_{12-x}Al_xO_{19}$ (x=2.2, 2.3, 2.4 and 2.5) M-type hexaferrite powders synthesized by sol-gel auto-combustion method

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Abstract

In this research, we report the synthesis, structural and microstructural studies of rare-earth free M-type hexaferrite powders with formula $Ba_{0.54}Ca_{0.46}Fe_{12-x}Al_xO_{19}$ (x=2.2, 2.3, 2.4 and 2.5), which were successfully prepared via the sol-gel auto-combustion method. The samples were annealed at a temperature of 1250 ◦C for 5 hours. X-ray diffraction (XRD) analysis showed that the samples have the M-type phase with no traces of any other secondary phase. Structural parameters such as lattice constants a and c, cell volume (V_c), crystallite size (D) and strain (ϵ) are discussed. Scanning electronic microscope (SEM) analysis revealed that the grain sizes of the samples decreased with the increase in Al^{3+} concentration. Energy dispersive X-ray (EDX) analysis confirmed the composition of the prepared powders as the theoretical atomic proportions of Ba, Ca, Fe, Al and O match well with the experimental values.

Investigation of the Physical Properties of Quaternary Heusler CsNaICl: A DFT Study

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Abstract

This study investigates the fundamental physical properties of the CsNaICl compound using density functional theory (DFT) calculations performed with the Wien2k software package. The analysis encompasses the structural, elastic, electronic, optical, and thermoelectric properties of the alloy. The studied material exhibits tetragonal symmetry, characterized by lattice parameters a_0 = 4.719 Å and c_0 = 7.736 Å. The Pugh's ratio of 2.1893, which is above the critical threshold of 1.75, indicates that the CsNaICl compound demonstrates ductile behavior. Additionally, this quaternary Heusler compound is found to be a non-magnetic insulator with an indirect band gap of E_g = 6.358 eV. Its optical properties, including a refractive index with static values of 1.46 along the zz direction and 1.51 along the xx and yy directions, as well as the extinction coefficient, absorption coefficient, and dielectric tensor components, exhibit excellent light transmission and strong photon interaction, highlighting its potential for advanced optical applications. The thermoelectric characteristics were examined through parameters such as the Seebeck coefficient, electrical conductivity, and thermal conductivity over a temperature range of 0–1000 K. These findings demonstrate the material's capacity for thermal-to-electrical energy conversion, providing valuable insights for optimizing thermal systems and improving the performance of thermoelectric devices.

Keywords: Quaternary Heusler; DFT; Elastic parameters; Electronic properties; Optical properties; Thermoelectric properties.

Theoretical Study of Magnetic, Magnetocaloric, and Hysteresis Behavior of the Antiperovskite Compound Mn3AlN

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Abstract

In this study, we explore the magnetic, magnetocaloric properties, as well as the hysteresis behavior of the antiperovskite compound using a theoretical approach based on the mean-field approximation. We examine the effects of the magnetic field and exchange interactions on the site magnetization, magnetic susceptibility, magnetic entropy change, as well as the hysteresis behavior of this material. The results show that undergoes a second-order magnetic phase transition, with a maximum magnetocaloric effect around the critical temperature. Moreover, the relative cooling power (RCP) increases monotonically with magnetic field strength, suggesting that this compound could be promising for magnetic refrigeration applications. Hysteresis behavior is also studied, revealing a decrease in coercivity and remanent magnetization with increasing temperature, until the hysteresis loop completely disappears above the critical temperature.

Revealing the optoelectronic properties of $AgMgX_3$ (X= F, Cl, Br) perovskites using density functional theory (DFT)

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Abstract

The search for new materials with interesting properties is crucial to the technological development of optoelectronic applications, including photovoltaic solar cells, photodetectors and light-emitting diodes. Using density functional theory (DFT), the structural, elastic, electronic, optical and phonon properties of cubic halide perovskites AgMgX3 (X = F, Cl and Br) have been investigated in the present work. The structural study showed that the equilibrium lattice constants for AgMgF3, AgMgCl3 and AgMgBr3 are 4.01 ˚A, 4.95 ˚A and 5.30 ˚A, respectively. Meanwhile, the thermodynamic stability of these materials has been confirmed by calculated formation energy values. In additions, the electronic properties showed a semiconducting character for the three studied compounds, with an indirect band gap (M -) of 1.95, 1.71 and 0.88 eV for AgMgF3, AgMgCl3 and AgMgBr3, respectively. The calculated elastic properties revealed the mechanical stability of the considered materials, as well as their ductile nature and anisotropic characteristics. Moreover, optical results showed that AgMgX3 (X = F, Cl and Br) materials absorb visible and ultraviolet radiations, making them suitable for a variety of applications, including photovoltaics and light-emitting diodes.

Exploring rare earth-based scintillators in advanced energy systems through Quantum ESPRESSO

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Abstract

Rare earth-based scintillators are essential components in advanced energy systems due to their exceptional luminescence properties and energy conversion efficiency. In this study, the structural, electronic, and optical properties of Rb LuCl and Rb $_{2}$ $_{5}$ $_{2}$PrCl$_{5}$ are investigated using Density Functional Theory (DFT) within the Quantum ESPRESSO framework. The analysis focuses on the relationship between their crystal structures and electronic configurations and their influence on bandgap energies and optical characteristics. The findings provide fundamental insights into the scintillation mechanisms of these materials, highlighting their potential for applications in radiation detection and high-energy physics. This work demonstrates the critical role of first-principles calculations in guiding the development and optimization of rare earth-based scintillators for advanced technological applications.

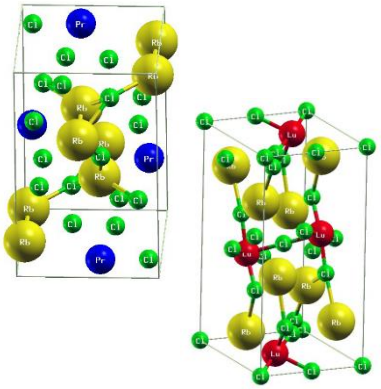

Figure 1: Crystal Structure of the Rare eath based scintillators

Keywords: Rare earth-based scintillators, Rb_2LuCl_5, Rb_2PrCl_5, Density Functional Theory (DFT), Quantum ESPRESSO, bandgap energy, optical properties, radiation detection, advanced energy systems.

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Grain Growth in Nanocrystalline Ni During Thermal Annealing: A Molecular Dynamics Study

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Abstract

Nanocrystalline materials have attracted significant research interest within the field of materials science, particularly nanocrystalline nickel. Thermal annealing, a fundamental topic of research, plays a critical role in determining the evolution of grain size in nanocrystalline metals. In this study, we investigate the isothermal grain growth behaviors of nanocrystalline nickel, focusing on the effect of annealing temperature. Molecular dynamics simulations using the Modified Embedded Atom Method (MEAM) potential developed by Lee et al. (3) were employed to provide detailed atomic-level information on the microscopic mechanisms involved in grain growth. Previous studies have demonstrated that annealing temperature has a significant impact on the grain growth of nanocrystalline metals. For instance, Simoes et al. (4) observed significant grain growth in nanocrystalline copper thin films with increasing annealing time and temperature. Chojnowski et al. (2) found that annealing nanocrystalline chromium at temperatures above 400◦C led to controlled grain growth. Chen et al. (1) reported a decrease in the frequency of annealing twins in highly rolled pure nickel as annealing temperatures increased. In this study, atomistic simulations were conducted to investigate the grain growth mechanisms, grain boundary structure, and the effects of annealing temperature on microstructural properties during grain growth. The models were constructed using the Voronoi geometrical method to study the grain growth mechanism. Our findings reveal that during thermal annealing, nanocrystalline nickel exhibits stacking faults, twinning, changes in grain size, rotations, and translations, which facilitate crystalline growth and grain coalescence. Grain boundary migration, grain rotation mechanisms, and dislocations (or stacking faults) were identified as intermediate mechanisms in the grain growth process. These results provide insights into how annealing temperature controls the rate of grain growth and its impact on the appearance of different types of defects during the growth.

Keywords: Thermal annealing, Nanocrystalline metals, Grain growth, Grain Boundaries, Nickel, Molecular dynamics

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Strain-engineered 2D h-BC2N monolayer as a potential gas sensor with exceptional sensitivity and selectivity for NO2 gas detection

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Abstract

Nitrogen-containing gases present notable threats to the human health and the environment, largely attributed to increased toxicity arising from industrial processes. This study assesses the reactivity of strained and unstrained h-BC2N monolayers towards NO2, NH3, and HCN gases using molecular dynamics simulations. The monolayer-gas interactions were analyzed by incorporating van der Waals dispersion correction. Biaxial gas adsorption energy notably increases across strain levels from –0.43 eV to –0.68 eV for 0 %–4 % strain, respectively. Conversely, NH3 and HCN show low adsorption energies on both strained and unstrained h-BC2N monolayers. Electronic analyses indicate the heightened sensitivity of NO2 compared to NH3 and HCN, with minimal sensitivity shown towards H2O, CO2, HF, H2, and H2S gases, suggesting high selectivity.

4) Intelligence artificielle

Influence of natural convection during solidification of binary alloy

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Abstract

Solidification of binary alloy is one of the most interesting domains in industrial applications, which has a variety of effects on the structural characteristics of metals. One critical aspect is the influence of natural convection throughout the process. In this work, we focus on the solidification behavior of a tin-lead (Sn-Pb) alloy, a widely used material in soldering and other industrial processes we conduct a comprehensive simulation to investigate the interplay between solidification and natural convection, offering insights that could pave the way for optimizing industrial processes and enhancing material performance.

Keywords: solidification, natural convection, heat transfer, binary alloy

Identification des dynamiques entre NAO et AMO par des techniques de machine learning

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Résumé

Dans cette étude, nous avons exploré les dynamiques entre les oscillations climatiques Nord-Atlantique (NAO) et Atlantique Multidécennale (AMO) en appliquant des techniques avancées de machine learning. Une première approche basée sur la régression linéaire a permis didentifier des relations globales entre les deux phénomènes. Par la suite, des techniques de régression sparse, telles que SINDy (Sparse Identification of Nonlinear Dynamics), ont été mises en oeuvre pour modéliser des interactions non linéaires complexes tout en réduisant le bruit et en sélectionnant les termes les plus significatifs. Les résultats montrent que les dynamiques entre NAO et AMO sont influencées par des composantes linéaires et non linéaires. L'approche SINDy, en particulier, a permis d'identifier des structures dynamiques sous-jacentes avec une grande précision, mettant en évidence des modèles explicatifs plus parcimonieux. Ces résultats ouvrent de nouvelles perspectives pour l'analyse des interactions climatiques et leur prévision à long terme.

Effects of nanoparticles on unsteady blood flow through artery having both stenosis and aneurysm with magnetic field and body acceleration

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Abstract

The study of blood flow in diseased arteries has been an important area of research in recent years. The most common arterial lesion in humans is stenosis/aneurysm generated by the accumulation of cholesterol plaque inside the vessel wall. The current work investigates the unsteady, laminar and two-dimensional pulsatile flow of non-Newtonian blood through an artery with stenosis and aneurysm, containing nanoparticles in the presence of body acceleration. Motivated by the magneto-hemodynamics effects, a uniform magnetic field was applied in the radial direction to the blood flow. A radial coordinate transformation is used to immobilize the effect of the vessel wall. The governing nonlinear partial differential equations of the present flow together with prescribed boundary conditions are discretized by employing explicit finite difference scheme. A computer code is developed, in order to solve these algebraic equations. Comprehensive solutions were presented for different nanoparticles mediated blood flow at both the stenosis and aneurysm segments. The analysis reveals that the applied magnetic field, periodic body acceleration and nanoparticles have considerable effects on the flow field and heat transfer.

Keywords: Blood flow, Heat transfer, Non-Newtonian, nanoparticles, Magnetic field, Stenosis, Aneurysm.

Entropy generation analysis of a hybrid nanofluid during free convection via two concentric cylinders partially filled with porous media and subjected to a magnetic field

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Abstract

The purpose of this study is to investigate the magneohydrodynamic heat transmission in a partially porous annular space between two coaxial cylinders with a permeable interface saturated by a hybrid nanofluid (water-Cu/Al2O3) and to investigate the entropy generation to better understand the heat transfer processes. The inner and outer cylinders are kept at a constant hot and cold temperature. The base walls are both impermeable and insulated. The Successive Over Relaxation (SOR) method is used to solve the nonlinear coupled conservation equations utilizing a vorticity-stream function based on finite differences. The numerical results obtained in terms of streamlines, isotherms, Nusselt and Bejan numbers, and entropy generation are presented to show the effect of various control factors. According to the results of this numerical simulation, increasing the Ra number improves thermal energy transfer across the active wall. In addition, the mean entropy generation elements increase with increasing Rayleigh number, Darcy number, and nanoparticle concentration; nevertheless, with the exception of magnetic irreversibility, the reverse development is seen. In addition, the Bejan number is decreased in order to raise the Rayleigh and Darcy numbers.

Keywords: Natural convection, Entropy generation, Hybrid nanofluid , magnetic field, Porous medium.

Quantum Synthetic Oversampling: A Novel Approach to Address Imbalanced Data Using Quantum Computing

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Abstract

Imbalanced datasets pose significant challenges in machine learning, often resulting in biased models that underperform on minority classes. This work introduces Quantum Synthetic Oversampling (Q-SMOTE), a quantum-enhanced method inspired by SMOTE, designed to generate synthetic samples for underrepresented classes. By leveraging amplitude encoding for data representation, quantum state interpolation for sample synthesis, and amplitude amplification to focus on boundary-relevant samples, Q-SMOTE efficiently balances datasets. We demonstrate the feasibility of this approach on small-scale quantum processors, showcasing its potential to revolutionize data preprocessing for imbalanced learning scenarios.

Analyse des Propriétés physiques des Schistes Bitumineux au Maroc

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Résumé

Dans ce travail, nous étudions la variabilité de la composition lithologique et de la teneur en matière organique des échantillons prélevés dans les différentes couches M, X et Y du schiste bitumineux de Timahdit au Maroc, dans le but d' analyser expérimentalement l'impact de cette variabilité sur les mesures thermo-physique. L'objectif de cette étude est de prédire les propriétés des couches, notamment leur diffusivité thermique, ainsi que les vitesses des ondes P et S. Les résultats de l'étude sur l' impact de la teneur en matière organique des échantillons sur les mesures thermo-physique montrent que, quelle que soit la teneur en matière organique, la diffusivité reste insensible, tandis que les vitesses des ondes P et S diminuent de manière linéaire avec l'augmentation de la teneur en matière organique. D'autre part, l'étude de la variabilité de la teneur en matière organique est cohérente avec le rapport des vitesses, pouvant ainsi être utilisée comme indicateur de la matière organique des couches. La diffusivité thermique est presque invariante face `a la variabilité de la teneur en matière organique.

Mots-clés : schiste bitumineux- Diffusivité thermique- vitesses des ondes P-vitesses des ondes S- Matière organique ‐ thermo-physique.

Quantum Whale Optimization Algorithm (QUWA) For Feature Selection In High-Dimensional Data

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Abstract

Feature selection is a crucial preprocessing step in high-dimensional data, as it involves identifying and retaining the most relevant features. Among the feature selection methods, wrapper methods select a subset of features based on the evaluation criteria of a learning algorithm. However, these methods are computationally costly, as the evaluation of each subset necessitates the training of the adopted classifier.

To address these computational challenges, this study proposes to enhance the performance of the classical Whale Optimization Algorithm (WA) by incorporating the principles of quantum computing. The Quantum Whale Optimization Algorithm (QUWA) method utilizes the Q-bit representation, the quantum rotation gate, and modified evolutionary operators such as selection, mutation, and crossover.

The efficacy of the QUWA method is evaluated and compared against the standard WA and well-established evolutionary, swarm, and quantum algorithms. The experimental results demonstrate the superior performance of the QUWA approach.

Keywords: (1) Quantum (2) Whale Optimization Algorithm (3) Feature selection

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IA et trous noirs

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Résumé

La théorie quantique des trous noirs soulève des questions fondamentales sur la nature de l'information dans l'univers. Le paradoxe de l'information des trous noirs, qui ´émerge du conflit entre la m´mécanique quantique et la relativité générale, reste une ´énigme majeure. Particulièrement, l'intérêt se porte sur les trous noirs `a quatre dimensions en présence d'un champ appelé quintessence, considéré comme un candidat de l'énergie noire. Pour comprendre son impact, une analyse analytique du spectre de la radiation ainsi que de l'aspect thermique des solutions chargées et rotatives est effectuée. Le rayonnement de Hawking, produit par des interactions quantiques `a l'horizon du trou noir, semble emporter uniquement des informations thermodynamiques, ce qui alimente ce paradoxe. Le machine learning (ML), et en particulier ses variantes avancées comme le deep learning et les réseaux neuronaux quantiques (QNN), offre des outils puissants pour analyser ces questions complexes. Dans ce contexte, le ML peut être utilisé pour modéliser l'entropie et l'information; les algorithmes non supervisés aident `a explorer les corrélations dans les données simulées du rayonnement de Hawking et `a quantifier la fa, con dont l'information est encodée ou transportée. L'intégration de ces approches avec l'informatique quantique ajoute une dimension supplémentaire, permettant de simuler les interactions quantiques `a l'échelle des qubits, de tester des théories comme la gravité quantique et d'explorer l'intrication quantique associée aux trous noirs. Ces avancées pourraient non seulement résoudre le paradoxe de l'information, mais également offrir des outils pour comprendre les principes fondamentaux de l'univers.

Analysis of Advanced Signal Processing Techniques for Blind Source Separation of EEG Signals

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Abstract :

This study provides an in-depth exploration of advanced signal processing techniques for EEG signals, with a particular focus on blind source separation and signal decomposition. The research is framed within a medical context, addressing brain anatomy and physiology, methods for measuring neural activity, and objectives related to EEG signal analysis. Specific challenges in this field, such as interferences and artifacts, are also discussed.

The methods examined include Independent Component Analysis (ICA) and approaches based on higher-order statistics for artifact removal. Denoising techniques, such as wavelet-based methods, are also reviewed. Additionally, decomposition methods like Empirical Mode Decomposition (EMD) and Variational Mode Decomposition (VMD) are studied, highlighting their fundamental principles and applications in enhancing the interpretation of EEG signals.

A rigorous experimental methodology was implemented to evaluate these approaches, and the results demonstrate their effectiveness in analyzing EEG signals, thereby contributing to a better understanding of cerebral processes and improving diagnostic tools.

Keywords: EEG signals, blind source separation, EMD, VMD

Communications par Affiche

First-principles Calculations to Investigate Structural, Electronic and Optical Properties of Rare Earth alloys

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Abstract

This manuscript analyzes the characteristics of rare earth materials XFe 5 (X = Sm, Dy, or Nd) with a focus on their structural, electronic, and optical properties using density functional theory (DFT) as implemented in the Wien2k software package. The exchangecorrelation potential is accurately described using the GGA+SOC+U method, which is particularly important for evaluating electronic and magnetic properties. XFe 5 materials exhibit metallic behavior, typical of ferromagnetic substances. In terms of optical characteristics, the study demonstrates high absorption in the ultraviolet (UV) region. The materials display different absorption capacities, with distinct curves and absorption peaks, indicating varied responses to UV exposure.

Combining Density functional theory and Monte Carlo simulation to Study the Electronic, Magnetic, and Magnetocaloric Properties of the quadruple perovskite CaCu3Fe2B2O12 (B=Re, Os and Ir)

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Abstract

In this study, the theoretical study of the CaCu3Fe2B2O12 (B=Re, Os and Ir) quadruple perovskite with ferrimagnetic mixed-spin is performed by combining both the density functional theory (DFT) and Monte Carlo simulations (MCs) based on the metropolis algorithm. We assessed the electronic structure, the band structure, the magnetic properties, and the magnetocaloric effect of the CaCu3Fe2B2O12 (B=Re, Os and Ir) compound. Based on the electronic density of states and electronic structure, it is found that the studied compounds are metallic materials. Computational magnetic results for two examined materials reveal the non-zero total magnetic moments. The exchange interactions parameters are calculated in order to perform the Monte Carlo simulation (MCS). The magnetic properties, magnetocaloric effect (MCE) and the relative cooling power (RCP) are also investigated. The results show that the compounds can be a promising candidate for magnetic refrigeration.

DFT investigation of the structural, optoelectronic, thermoelectric, and thermodynamic properties of metal phosphides MP2 (M = Co, Rh, and Ir)

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Résumé

Materials science is concerned with the development of novel materials that possess specified physical characteristics. In this work, we study MP2 (M = Co, Rh, Ir) compounds which crystallize in the monoclinic structure with formation energy equal to -11.72eV, -11.62, and -11.13 for CoP2, RhP2, and IrP2, respectively. These materials in high temperature present an important advance for thermoelectric applications. First-principles calculations with density functional theory (DFT) are employed to investigate the electrical, optical, thermoelectric, and thermodynamic properties of MP2 (M = Co, Rh, and Ir) compounds. All computations are performed using density functional theory (DFT) and the Wien2K method. By combining the modified BeckeJohnson of Tran-Blaha potential (TB-mBJ) with the approximated gradient generalized (GGA), the precision of the restricted band has been optimized. This approach, in conjunction with tools like GIBBS2 and Boltzmann's theory of transport, has made it possible to ascertain the thermodynamic and thermoelectric properties of the materials under study. The results show that these materials have a straight band gap of CoP2 is 4.78 eV, whereas the indirect band gaps of RhP2 and IrP2 are 0.575 eV and 0.875 eV, respectively. The optical characteristics indicated good optical absorption and conductivity in the ultraviolet and visible ranges. Furthermore, using Boltzmann's theory, It was revealed that the figure of merit ZT is more than 1.7 at a temperature of T = 700K, notably for CoP2. In fact, our study demonstrates that MP2 (M = Co, Rh, and Ir) compounds might be effective in ultraviolet and visible photoelectric applications, as well as thermoelectric applications.

Compact and Miniaturized Super Broadban Antenna Based on Textile Substrate for Potential Electromagnetic Energy Harvesting and Other Applications

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Résumé

In the current study, a compact, super-wideband flexible textile antenna is designed to operate across an exceptionally broad frequency range from 3.16 to 50 GHz. The antenna features a straightforward geometry with an offset rectangular patch incorporating three slots to enhance performance, complemented by a circular parasitic patch on the opposite side of the substrate. Fabricated on a footprint of 30 mm × 25 mm × 1 mm, the antenna exhibits electrical dimensions of 0.31λ × 0.26λ × 0.012λ at 3.16 GHz. The antenna's performance is evaluated using CST Microwave Studio 2019® software. Measurement results demonstrate a wide bandwidth of 15.82:1, spanning from 3.16 to 50 GHz, with a peak gain of 7.70 dBi at 23.05 GHz. An equivalent circuit model of the antenna is developed and analyzed using ADS software. The antenna's performance is further assessed by investigating the effects of structural bending and proximity to the human body. Importantly, the antenna maintains acceptable levels of specific absorption rate (SAR), ensuring compliance with safety standards for RF exposure. Experimental measurements closely corroborate simulated outcomes. Given its uncomplicated topology, compact dimensions, super-wideband characteristics, and high gain, the antenna is well-suited for low-power applications in practical scenarios.

Quantum entanglement and measurement

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Résumé

Quantum information theory provides a framework for understanding the fundamental principles of quantum mechanics and their applications in information processing. A central concept in this field is quantum entanglement, a phenomenon in which the quantum states of two or more particles become interconnected such that the state of one particle instantaneously influences the state of the other, regardless of distance. This project explores the intricate relationship between quantum entanglement and quantum measurement, focusing on key concepts such as entropy, Bell inequalities, and the EPR paradox. We examine the role of von Neumann and R´enyi entropies in quantifying the degree of entanglement within a quantum system, providing insight into the amount of information required to describe the system's state. Furthermore, we investigate how Bell inequalities serve as a tool for distinguishing between classical and quantum correlations, thereby demonstrating the non-classical nature of entanglement. The EPR paradox is also analyzed to illustrate the counterintuitive implications of quantum mechanics and its impact on our understanding of reality. This study aims to deepen our comprehension of quantum entanglement and measurement, offering a thorough analysis of the theoretical frameworks and experimental validations that underscore these phenomena. By elucidating these concepts, we contribute to the broader discourse on the potential applications and implications of quantum information theory in advancing technology and fundamental science.

Improvement in phase sensitivity of the SU(1,1) interferometer through Kerr state seeding

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Abstract

A coherent seeded SU(1,1) interferometer represents a significant advancement in precision measurement methodologies. In this study, we theoretically investigate the phase sensitivity of an SU(1,1) interferometer seeded with a Kerr state, analyzing its performance under both single intensity and homodyne detection schemes. To establish the lower bound for phase sensitivity, we calculate the quantum Cramér-Rao bound through the quantum Fisher information approach. Our findings indicate that, under certain conditions, Kerr state seeding achieves superior phase sensitivity compared to traditional vacuum and coherent seeding approaches. These results suggest that Kerr states may serve as promising non-classical alternatives in the domains of quantum information and sensing technologies.

Etude de certaines propriétés physiques du Co2MnGe Heusler : calcul DFT et simulation Monte Carlo

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Résumé

Dans ce travail, nous avons utilisé la méthode des premiers principes basée sur la théorie de la fonctionnelle de la densité (DFT) pour étudier la structure électronique, la densité d'états, la structure de bande et les couplages d'échange du composé de Heusler Co_2MnGe. Les propriétés magnétiques de ce matériau ont été étudiées à l'aide de simulations de Monte Carlo (MCS) dans le cadre d'un modèle d'Ising tridimensionnel. En particulier, nous avons évalué l'aimantation, la susceptibilité magnétique, la chaleur spécifique et le cumulant de Binder et calculé certains exposants critiques du système. Les résultats ont montré que le composé de Heusler Co_2MnGe présente un comportement semi-métallique et subit une transition de la phase ferromagnétique à la phase paramagnétique à une température critique $T_c \approx 990$ K, en bon accord avec les données expérimentales. Les valeurs des exposants critiques calculés sont très similaires à celles connues pour le modèle d'Ising tridimensionnel : $\alpha \approx 0.1191$, $\beta \approx 0.3188$, $\gamma \approx 1.2526$, et $\nu \approx 0.5526$, vérifiant le comportement universel du système étudié.

Mots clés : Théorie De La Fonctionnelle De La Densité, Simulation De Monte Carlo, Co_2MnGe Heusler, Propriétés Electroniques, Propriétés Magnétiques, Modèle d'Ising, Exposants Critiques.

Abstraction graphique

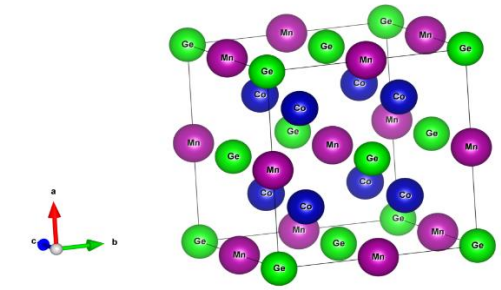

Figure 1 *: Structure cristalline du Co_2MnGe Les sphères violettes représentent les atomes de manganèse, les sphères bleues les atomes de cobalt et les sphères vertes les atomes de germanium.*

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Investigation of electronic, thermodynamic, and optical properties of LiTi2O4 cathode material for Li-ion battery: An Ab Initio calculations

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Abstract

In this research, we have conducted an in-depth investigation into the structural, electronic characteristics, and thermodynamic properties of the LiTi2O4 compound using first-principles calculations grounded in density functional theory with the generalized gradient approximation. Our findings reveal that the LiTi2O4 compound possesses a calculated lattice constant of 8.407 Å. Furthermore, we have derived critical battery-related properties, including an average voltage of 1.53V versus Li/Li + and an energy density of 245 Wh/kg. To deepen our understanding of LiTi2O4 , we have explored its thermodynamic properties employing the quasi-harmonic Debye model. These properties encompass the Debye temperature, volume variation, compressibility modulus, specific capacity, and thermal capacity. Importantly, we have observed that the Debye stiffness of LiTi2O4 increases with rising pressure. Moreover, we have conducted measurements to assess various optical properties of the LiTi2O4 compound. These properties include the absorption coefficient, photoconductivity, and reflectivity.

Keywords: LiTi2O4 ; Li-Battery; DFT; Average voltage; Absorption coefficient, photoconductivity, and reflectivity.

AI-Assisted 2.7 µm Lasing in Er^{3+}-Doped Tellurite Fiber Lasers with Different Pumping Schemes

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Abstract

The laser performance of Er^{3+}-doped tellurite fiber lasers operating at 2.7 µm, based on the ${}^4I_{11/2} \rightarrow {}^4I_{13/2}$ transition, has been theoretically studied using propagation equations combined with AI-based optimization techniques. Artificial intelligence was employed to systematically investigate the effects of pumping configuration and fiber length on output power, as well as intracavity pump and laser power distributions. This approach allowed for the optimization of fiber laser performance. Under a pump power of 20 W, the maximum slope efficiency (27.62%) and maximum output power (5.219 W) were predicted for different fiber lengths (1 m, 3 m, and 5 m) across three pumping configurations.

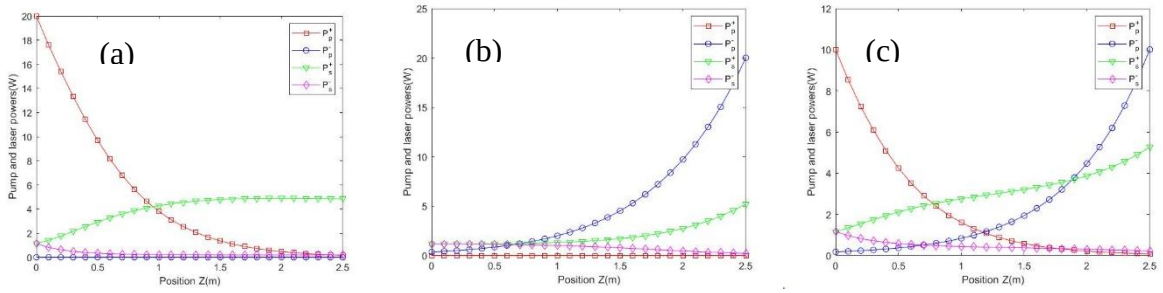

Figure 3 – The distribution of pump and laser powers along the fiber length (a) in forward pumping configuration, (b) in backward pumping configuration, (c) in bi-directional pumping configuration

Keywords: Tellurite fiber laser, Er3+-doped fiber, Pump scheme, The output power, Pump and laser power distributions, slope efficiency, fiber lengths.

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Exploring the structural, electronic, and optical properties of CaGa2X4 (X = S, Se) chalcogenide spinels for potential solar cell applications: DFT study

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Abstract

The main purpose of this study is to explore the structural, electronic and optical properties of CaGa2X4 (X = S, Se) materials for their applications in solar cells, using density functional theory (DFT) calculations in Wien2K software. Structural properties reveal that both compounds possess a cubic phase with the space group Fd-3m (n◦227). The stability of both compounds is verified by the negative formation energy. Band structure calculations, using the modified Becke-Johnson potential (TB-mBJ), indicate that CaGa2S4 and CaGa2Se4 possess direct band gaps of 1.956 eV and 1.120 eV for CaGa2S4 and CaGa2Se4, respectively. Optical properties are examined via absorption, optical conductivity, dielectric function, optical bandgap and Urbach tail. These calculations indicate significant absorption and optical conductivity in the visible range for both materials. Overall, these results suggest that CaGa2X4 (X = S, Se) chalcogenide spinels are promising as candidate materials for solar cell applications.

Quantum Neural Networks in Tumor Classification

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Résumé

Une classification précise des tumeurs est essentielle pour un diagnostic efficace et la planification des traitements en oncologie. Les modèles traditionnels d'apprentissage automatique ont montré des résultats prometteurs, mais ils se heurtent souvent à des limitations lorsqu'il s'agit de traiter des données d'imagerie médicale complexes et de haute dimension. Cette étude présente l'utilisation des Réseaux Neuronaux Quantiques (QNNs) comme un outil de calcul avancé pour la classification des tumeurs, exploitant les capacités uniques de l'informatique quantique pour relever ces défis.

Spin polarized effects on Physical Properties of double Perovskite Materials for Spintronic and Thermoelectric applications

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Abstract

FP-LAPW method is utilized to explore the spin polarized effects on structural, electronic, magnetic, and thermoelectric properties of new cubic X2CeVO6 (X=Sr, Ba) double perovskite oxides. The tolerance factor and elastic parameters show and ensure the stability and formation of both perovskites in the cubic phase. Additionally, the predicted mechanical constants show that X2CeVO6 (X=Sr, Ba) behave as stable ductile materials. Then, spin-polarized calculations show ferromagnetic and half-metallic behavior for both compounds with a total magnetic moment equal to 1 μβ. Thermoelectric parameters of both materials show high power factor and n-type conductivity, due to the multiple oxidation states of Vanadium. Therefore, these results show that the proposed perovskites X2CeVO6 (X=Sr, Ba) can be promising materials for spintronic and thermoelectric applications.

Role of Substitutional Sb-doping on Stability Structural, Half-metallicity, Elastic, Electronic and Magnetism of Co_2MnSn Full Heusler Compound

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Abstract:

Density Functional Theory (DFT) calculations were performed using the full potential linearized augmented plane wave method to adjust the Fermi level by doping Co_2MnSn with Sb. This was done through the Generalized Gradient Approximation (GGA) and modified Becke-Johnson (mBJ-GGA) formalisms to enhance spin polarization and suggest signs of half-metallicity. For both ferromagnetic and paramagnetic phases, lattice optimization was performed to identify the stable magnetic structure. The results designate that the doped alloys are stable in a ferromagnetic phase with an $L2_1$ structure. The calculated elastic constants suggest that the doped alloys meet the criteria for mechanical stability. The magnetism in these compounds is primarily due to the localized moments on the Mn and Co atoms. According to mBJ-GGA calculations, the total magnetic moment slightly increases with Sb doping. Analysis of the optical constants revealed the optoelectronic properties, confirming semiconducting behavior. Doping elements to achieve half-metallicity is demonstrated to be an effective method for discovering new materials suitable for spintronics applications.

Keywords: DFT, Half-metallic, Ferromagnetic, Elastic constants, Optoelectronic characteristics

RELATIONSHIP BETWEEN CHEMICAL DURABILITY, STRUCTURE, AND THE IONIC-COVALENT CHARACTER OF P-O-Me BOND (Me = Pb, Fe), IN THE VITREOUS PART OF THE TERNARY SYSTEM Fe2O3-PbO-P2O5 GLASSES

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Abstract

Phosphate based materials are today the subject of many studies for their use in the confinement of harmful waste. Glasses of phosphates containing iron and lead were produced by direct melting at 1080-1100 °C. The study of the dissolution rate carried out on synthesized glasses, immersed in distilled water at 90 °C for 30 days, indicates considerable chemical durability. The increase in the content of Fe2O3 in the glass network, at the expense of PbO, is a favorable factor for chemical durability. Different techniques have been used such as DSC, X-ray diffraction, infrared spectroscopy IR, MEB, and density. These studies have established correlations between chemical and structural properties.

Keywords: Phosphate glasses, Density, IR, XRD, Chemical durability, Vitrification, Radioactive waste.

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Overview of Energy Storage techniques: addressing Materials and Manufacturing Challenges

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Abstract

Energy storage systems are crucial to meeting the growing demand for reliable, sustainable, and efficient energy solutions. The development of next-generation energy storage technologies depends heavily on the discovery and integration of innovative materials. These advancements in materials contribute significantly to the development of high-capacity energy storage devices, making them more suitable for applications in renewable energy storage. In this work, we provide a comprehensive examination of energy storage systems, focusing on the technological, material, and manufacturing challenges involved in their development, deployment, and potential for widespread adoption.

Entanglement within a graphene layer with a scattering process under thermal fluctuations

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Abstract

Cutting-edge quantum processing technology is currently exploring the remarkable electronic properties of graphene layers, such as their high mobility and thermal conductivity. Our research is dedicated to investigating the behavior of quantum resources within a graphene layer system with a scattering process, specifically focusing on quantum correlations, while taking into account the influence of thermal noise. To quantify the amount of entanglement, we use logarithmic negativity (LN). We examine how factors like temperature, inter-valley scattering processes strength, and other system parameters affect entanglement in graphene. Our results reveal that higher temperatures lead to a reduction in LN within graphene layers. By optimizing system parameters such as band parameter, wavenumber operators and scattering processes strength, we can mitigate the impact of thermal noise and enhance the quantum advantages of graphene-based quantum processing.

Comparative Analysis of Reflectivity and Pumping Schemes on the output power of Tm^{3+}-Doped Fiber Lasers at 1.72 µm

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Abstract

In this study, we revealed the impact of pumping scheme, fiber length, pumping power, and the reflectivity of the output fiber Bragg grating on the performance of a Tm3+ -doped fiber laser (TDFL) operating at a wavelength of 1.72 μm. Numerical simulations enabled the optimization of output power and the reduction of losses due to reabsorption as well as amplified spontaneous emission (ASE) around 1820 nm. The Tm3+-doped fiber was bi-directionally pumped at 1570 nm to enhance pump absorption. The simulations suggest that a maximum power of 5.96W at 1.72 μm and a slope efficiency of 64% are achievable using a Tm^{3+}-doped silica fiber with a bi-directional pump of 4 W forward and 6 W backward.

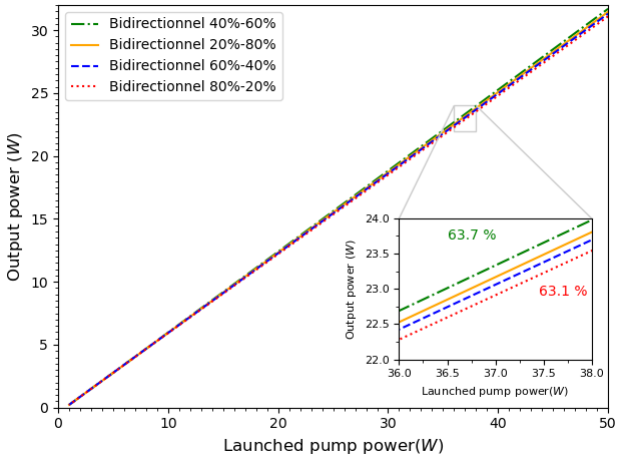

Figure : Output power calculated at 1720 nm as a function of lunched pump power at 1570 nm. (with zoom in the inset)

Keywords: Thulium doped fiber lasers, Rate equation, Amplified spontaneous emission (ASE), 1.72 μm, Pump scheme

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Structural and optical properties of Eu_2O_3-ZnO composite prepared by solid state method.

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Abstract

The Eu_2O_3-ZnO composite synthesized through solid-state method, was characterized using X-ray diffraction (XRD) and UV-Visible spectroscopy to assess its structural and optical properties. Rietveld analysis confirmed the coexistence of Eu_2O_3 and ZnO phases, with weight percentages of 75.44(1.27) % and 24.56(1.15) %, respectively. The lattice parameter of Eu_2O_3 was determined to be a=10.866(1) Å, while ZnO exhibited lattice parameters of a=b=3.249(1) Å and c=5.20489(5) Å. The absorbance spectra of the composite material indicated band gaps of 3.20 eV and 3.79 eV, corresponding to those of ZnO and Eu_2O_3, respectively.

Keyword: XRD analysis; UV-Visible spectroscopy; composite; optical band gap.

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Aluminum Substitution Effects on the Structure and Morphology of $SrFe_{12-x}Al_xO_{19}$ Hexaferrites

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Abstract

The impact of aluminum substitution on the structural and morphological properties of $SrFe_{12-x}Al_xO_{19}$ (x = 1, 1.5, 2 and 2.5) hexaferrite powders synthesized via the sol-gel auto-combustion method was investigated. Rietveld refinement of X-ray diffraction data confirms a hexagonal structure and reveals a progressive decrease in lattice parameters a, b, and c with increasing aluminum content, attributed to the smaller ionic radius of Al^{3+} compared to Fe^{3+}. Scanning Electron Microscopy (SEM) analysis shows well-defined grain morphology, with observable changes in particle size and distribution correlated to the substitution level.

Keywords: Hexaferrites, Aluminum substitution, Sol-gel auto-combustion method, Rietveld refinement, Scanning Electron Microscopy (SEM)

Studying quantum coherence and non-classical correlations in two non-interacting two-level atoms within thermal reservoirs

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Abstract

This paper delves into the exploration of quantum resources within a two-qubit system composed of two 2-level atoms connected to distinct thermal baths. Various quantifiers are employed to evaluate different aspects of the system's quantum characteristics. Specifically, the ‘1-norm and relative entropy of coherence are utilized to gauge quantum coherence, while local quantum Fisher information (LQFI) is used to quantify non-classical correlations within the system. The findings suggest that the amount of quantum correlations and coherence decline as the spontaneous emission rate and the mean thermal photon number n increase. However, it is observed that manipulating parameters defining the initial state of the two-level atoms system can enhance non-classical correlations and quantum coherence between the two atoms. Additionally, it is noted that these three key metrics entirely vanish in the asymptotic limit of time. Our research underscores the importance of precisely adjusting the parameters of the initial system state, which is prepared in an extended Werner-like state (EWL), to protect quantum resources shared between the two atoms from environmental influences.

Keywords: Local quantum Fisher information; quantum coherence; Werner-like (EWL) state; 2-level atoms; thermal baths.

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Pressure-Driven Intrinsic Quantum Confinement and Semiconducting-to-Metallic Transition in the Topological Flat Bands Kagome Nb_3Cl_8 compounds

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Abstract

Nb_3Cl_8 is a unique subset of two-dimensional (2D) crystalline materials renowned for their Kagome structure and distinctive flat energy bands. These bands contribute to the distinct electronic behavior, rendering Nb_3Cl_8 a compelling subject for study. In this study, by employing *ab-initio* calculations, we scrutinize the impact of pressure on the electronic properties of Nb_3Cl_8, yielding valuable insights. Under high pressures, Nb_3Cl_8 undergoes a transition from a semiconductor state (with a 1.23 eV bandgap) to a metallic one, accompanied by electronic band restructuration. Notably, the flat energy bands were suppressed with increasing pressure. Furthermore, our investigation underscores the distinctive nature of flat energy bands in Nb_3Cl_8, delving into quantum effects, particularly their association with the quantum confinement of electronic states. The confinement of charge carriers in Nb_3Cl_8 results in discrete energy levels, corresponding to specific orbitals in the density of states, indicating robust electron confinement. Pressure-induced changes in the energy gap between these quantized levels suggest a decrease in confinement strength. Consequently, our study lays a robust foundation for future exploration, contributing to the development of innovative electronic devices grounded in quantum confinement effects.

Keywords: Flat bands, Quantum confinement, phase transition, applied pressure, electronic properties

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Computational Strategies in Radiation Dosimetry: Evaluating Monte Carlo and MIRD Calculation Methods

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Abstract

The Monte Carlo method and the method proposed by the Medical Internal Radiation Dose (MIRD) committee are among the most widely used methods for estimating absorbed dose in nuclear medicine. In fact, The MIRD committee is a committee of the Society of Nuclear Medicine, set up in 1965 to develop methods, models, assumptions and a standard mathematical scheme for assessing the internal radiation doses of administered radiopharmaceuticals. The organ-based approach to MIRD dosimetry uses organ-level S-factors, which represent the average absorbed doses in the target organs per unit of activity in the source organs. S values are tabulated for a large number of radionuclides and geometric combinations ranging from the sphere to anthropomorphic descriptions.

The Monte Carlo method is very useful as it takes into account the complexity of to take into geometric models and the different radionuclide emissions. In what follows, we compare the two, focusing on the calculation of absorbed doses to target organs.

Keywords : internal dosimetry, Monte Carlo, Medical Internal Radiation Dose.