Université Mohammed V
Faculté des Sciences
Rabat

ENSA
المدرسة الوطنية للعلوم التطبيقية بالجديدة
Ecole Nationale des Sciences Appliquées

المدرسة العليا للتربية و التكوين
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Ecole Supérieure d'Education et de Formation

جامعة شعيب الدكالي
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Université Chouaïb Doukkali

International Conference on Frontiers in Quantum Simulation, Applied Physics & Energy Innovation (ICQPEI 2025)

ENSA-EL JADIDA 18-19 DECEMBER 2025

Abstract Booklet

CNRST

INTERNATIONAL YEAR OF Quantum Science and Technology

RNJCS
Réseau National des Jeunes Chercheurs en Sciences

Conference Description

The first edition of this multidisciplinary conference was held from December 18-19, 2025 at the National School of Advanced Sciences, El Jadida (ENSA-UCD). It offers a forum for physicists and innovators, exploring the intersection of quantum physics with quantum information science, high-energy physics, applied physics, materials science, artificial intelligence, and energy innovation.

By connecting fundamental science and emerging technologies, the event aims to unite scientists, engineers, and professionals from a wide range of fields to explore and present cutting-edge advances in these thriving areas. The scientific program will feature invited talks by prominent specialists, contributed talks, and poster presentations.

All participants are strongly encouraged to present their work, which may cover a wide range of topics, including quantum information theory, quantum networks and the foundations of quantum physics, materials science (both numerical and experimental approaches), quantum many-body systems, non-equilibrium quantum statistical mechanics, advances in particle physics, astrophysics and cosmology, medical physics and artificial intelligence, as well as innovative technologies for the sustainable use of energy resources.

Invited Speakers

International Conference on Frontiers in Quantum Simulation, Applied Physics & Energy Innovation (ICQPEI 2025)

EL JADIDA 18-19 DECEMBER 2025



Pr. Hamid Nebdi
(Univ. Chouaïb Doukkali,
El Jadida, Morocco)

Speaker

Hamid Nebdi obtained his PhD in Atomic Physics (2000) and DEA in Physics (1997) from the Université Catholique de Louvain (Belgium), after advanced and undergraduate studies at Université Hassan II and Université Chouaïb Doukkali (Morocco). He joined the Royal Meteorological Institute of Belgium in 2001 as Research Assistant and became Acting Head of the Ionospheric Profiles Section in 2003. He contributed to major international projects such as ESA's Space Weather Pilot Project and Galileo Joint Undertaking, and represented Belgium in several COST management committees and ESA working groups. He later served four years as Assistant Professor of Physics at Umm Al-Qura University (Saudi Arabia), where he co-founded a Simulation Laboratory and initiated projects funded by KACST and the Saudi Ministry of Higher Education. Since 2018, he has been Director of the Laboratory of Innovation in Science, Technology and Modeling, and Professor at the Faculty of Sciences, El Jadida, where he coordinates the Master in Computational Physics and serves on the faculty council. His research spans radiation–matter interactions, ionospheric and space weather physics, atomic and laser physics. He has published widely, chaired international conferences, reviewed for leading journals, and is a member of several scientific societies (APS, ETPP21, SPANET, Société Belge de Physique, etc.). Active in academic and community service, he has presided multiple times over student and cultural associations in Belgium and Morocco.

Title: Space Weather: Toward the Forecasting of Geomagnetic Storms

Abstract: Solar activity refers to all the changes occurring in the Sun's magnetic field and atmosphere. These variations result from internal solar processes, particularly the movement of plasma and magnetic fields within the Sun. Solar activity takes many forms, including solar flares, sunspots, coronal mass ejections, and the solar wind. When these phenomena occur, they disturb Earth's magnetic field (the magnetosphere), producing geomagnetic storms of varying intensities. In this conference, we will introduce a new discipline currently developing in Morocco, dedicated to the study of these phenomena and their interactions with our biosphere: space weather. We will focus specifically on the study of geomagnetic activity through the planetary Kp index under extreme event conditions (major and severe storms). During such extreme events, Earth's environment and our technologies—both in space and on the ground—are affected by geomagnetic disturbances. To mitigate potential risks to technology during these events, a statistical analysis was carried out using a large dataset of Kp index values to identify geomagnetically active days over the last five solar cycles (20th to 24th).The evolution of the monthly occurrence probabilities across these solar cycles shows that these probabilities are higher during certain months than others. A significant correlation between the Kp index and sunspot numbers will also be highlighted.

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Université Chouaïb Doukkali

International Conference on Frontiers in Quantum Simulation, Applied Physics & Energy Innovation (ICQPEI 2025)

EL JADIDA 18-19 DECEMBER 2025



Pr. Mourad TELMINI
(Univ. Tunis El Manar, Tunisia)

Speaker

Mourad Telmini is Full Professor of physics at the Faculty of Sciences in Tunis (University of Tunis El Manar) and director of the Laboratory for Atomic and Molecular Spectroscopy & Applications (LSAMA). He holds a PhD in Atomic Physics from the University of Paris-Sud. He teaches quantum mechanics, atomic physics and quantum information in undergraduate and master's degrees. His research activities concern atomic physics (cold atoms and Bose-Einstein condensates in optical networks) and molecular (Rydberg states, halfium model, coherent control by ultra-short laser pulses). More recently, he has started research in quantum computing (variational calculus with quantum algorithms). He has published dozens of articles in international journals and has participated as a guest speaker at several international conferences. He is visiting professor at several universities in France, Germany, Brazil, South Africa, etc. He has held the positions of Director General of the National Centre for Nuclear Sciences and Technologies (CNSTN), and Vice President of the African Commission on Nuclear Energy (AFCONE). He represents Tunisia in the International Union of Pure and Applied Physics (IUPAP) on behalf of the Tunisian Society of Physics (STP), of which he is Vice-President, and currently chairs the Tunisian Association of Metrology (ATMET). He is also editor of the magazine African Physics Newsletters and co-head of the Tunisian quantum network QUANTUN, representing Tunisia in the international World Quantum Day network

Title: Introduction to Quantum Computing

Abstract: Quantum Computing is one of the most trending and promising chapters of all quantum technologies. The basic idea behind its development is the possibility to rely on the quantum properties of matter at the microscopic scale, mainly quantum superposition and quantum entanglement, in order to build up computing hardware (quantum circuits) and software (quantum algorithms) that can handle complex problems which are out of reach of conventional computing resources, within a reasonable amount of time. Quantum superposition has been demonstrated a long time ago and routinely used in several applications such as atomic clocks and interferometry, using, inter alia, the basic Rabi oscillations phenomenon. However, quantum entanglement was by far a more elusive phenomenon that has required significantly more effort from the physics community to provide fully accepted evidence of it. This field was triggered by the groundbreaking experimental work of A. Aspect in the 1980's, which demonstrated the violation of Bell's inequalities and proved the existence of quantum entanglement. Further research conducted by A. Zeilinger and others was able to implement quantum teleportation, based on quantum entanglement, opening up the possibility of effectively considering technological applications of these quantum properties. In this talk, I will present an overview of Quantum computing, including state-of-the-art developments. Then, I will demonstrate the power of quantum algorithms in the case of quantum cryptography, based on the Quantum Key Distribution (QKD) protocol. Furthermore, In will say a few words on the research that we are conducting in the laboratory of Atomic and Molecular Spectroscopy & Applications (LSAMA) in the field of hybrid algorithms, like the Variational Quantum Eigensolver (VQE), and their use in the electronic structure calculations in atomic and molecular physics.

International Conference on Frontiers in Quantum Simulation, Applied Physics & Energy Innovation (ICQPEI 2025)

EL JADIDA 18-19 DECEMBER 2025



Pr. El Kebir HLIL
(Institut de Néel de Grenoble, France)

Speaker

El Kebir HLIL is a Professor of Materials Science at the Néel Institute in Grenoble, France. From Teaching experience point of view, He is a lecturer of Physics of solids and Science of Material including synthesis, characterizations, measurements and simulations of physical properties Also, He is an international lecturer in the field of materials for conversion and storage energy. His research activity includes namely investigation on materials for storage and conversion of energy such as Metal hydrides, Thermoelectric materials, Magnetocaloric materials. For all investigated materials, special attention is paid to the industrial applications. He has participated in several International Schools as lecturer of electronic structure calculations, characterization as well as materials for energy. He is the most cited scientist in the world in the field of Magnetocaloric Ceramics. He supervised over 70 PhD students. He contributed to over 900 conferences and He published more than 800 papers in international learned journals.

Title : Matériaux magnétocaloriques pour la réfrigération éco-énergétique

Abstract:

La réfrigération magnétique, fondée sur l'effet magnétocalorique, constitue une alternative durable et éco-énergétique aux systèmes de réfrigération conventionnels. Ce travail porte sur le développement et la caractérisation de nouveaux matériaux magnétocaloriques, visant à obtenir un effet magnétocalorique élevé à température ambiante, une faible hystérésis et une bonne stabilité fonctionnelle. Une approche combinant la synthèse des matériaux, des caractérisations structurales, magnétiques et thermodynamiques, ainsi que la modélisation théorique, est adoptée afin d'optimiser leurs performances et d'évaluer leur potentiel d'intégration dans des dispositifs de réfrigération magnétique.



Pr. Pierre LACHKAR
(Institut de Néel de Grenoble, France)

Speaker

Professor Pierre LACHKAR, a lecturer and researcher at the Néel Institute (CNRS, Grenoble), has extensive experience in developing temperature sensors (thin layers structured on a suspended membrane). He currently manages a commercial cryostat, the Quantum Design PPMS (Physical Property Measurement System). This cryostat utilizes innovative technology to perform various material measurements down to very low temperatures (0.35 K) and under high magnetic fields.

Title : Advanced technologies for measurements of energy material properties

Abstract:

Recently, the PPMS is revealed as a performing system allowing numerous measurements of energy material properties such as magneto-resistance, specific heat capacity, electronic transport versus temperature and/or magnetic field under given vacuum. Mainly, this equipment allows Seebeck coefficient, electrical conductivity as well as heat conductivity requested for thermo-electricity investigations. Specific heat capacity measurements versus temperature under magnetic field can be performed as well. In addition, Hall effect measurements can be carried out. During my talk, adequate preparations including electrical connections will be explained and optimized methods for improved measurements will be debated. An available solution for labs to overcome difficulties with liquid helium supply will be presented. All these available datas will be discussed in terms of energy material efficiency.

International Conference on Frontiers in Quantum Simulation, Applied Physics & Energy Innovation (ICQPEI 2025)

EL JADIDA 18-19 DECEMBER 2025



Pr. Mohammed Khenfouch,
(Univ. Ibn Zohr, Agadir, Morocco.)

Speaker

Professor Mohammed Khenfouch, is a nanomaterials scientist and professional Physicist, originally from the North African country of Morocco, holds an undergraduate degree in solid-state physics, from the University Sidi Mohamed Ben Abdellah (USMBA) of Fez, Morocco. His keen interest led him to complete doctoral studies in Physics at the same university, which culminated in a Summa Cum Laude merit award for his novel research on optoelectronic applications. His interest in this field took flight during his MSc studies (Master in physics of materials and nanostructures) and has persisted till now, after he completed his PhD studies in July 2013, in the group of polymers and nanomaterials of the USMBA with a thesis titled: Elaboration and Physical and chemical studies of Graphene based nanocomposites for optoelectronic applications. His PhD study involved nanocomposites and devices for energy and optoelectronic applications inc. Solar cells, LEDs and Gas sensors. His active involvement in nanoscience research has helped him to gain a broad level of expertise and knowledge in materials science, especially in nanocharacterization and nanofabrication techniques with a deep practice in the fields of energy efficiency and nuclear waste management. In an attempt to take part in the fascinating nanoworld, and to contribute to its ambitious challenges, Mohammed undertook a postdoctoral position within the UNESCO-UNISA AFRICA Chair in Nanosciences and Nanotechnology at the College of science, engineering and technology of the University of South Africa. After two years, he worked in the department of physics of UNISA as a senior researcher and lecturer. During such period he has been a research visitor of world class teams and laboratories from many countries like Sweden, France, Spain, Canada, etc... Now, he is a professor in the faculty of applied sciences of the university of Ibn Zohr in Morocco. His large international network allows Professor Mohammed Khenfouch to be involved in many national and international research projects and be an active member of many societies and networks.

Title : Nanotechnology Horizons: Shaping Tomorrow with the World's Thinnest Industry

Abstract: Nanotechnology is redefining the limits of science and engineering by enabling control at the atomic and molecular scale. As the world's thinnest industry, it is not only shrinking dimensions but also expanding possibilities across medicine, energy, water treatment, electronics, and sustainable manufacturing. This presentation examines the latest breakthroughs in nanomaterials, nanoscale devices, and fabrication techniques, with a focus on how they are converging to address global challenges such as clean energy, resource efficiency, and environmental resilience. Beyond technical advances, we will explore the societal and ethical dimensions of nanotechnology, including safety, regulation, and equitable access. By mapping both the opportunities and the responsibilities that come with nanoscale innovation, this talk highlights how nanotechnology is poised to become a cornerstone of the next industrial and scientific revolution.

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EL JADIDA 18-19 DECEMBER 2025



Dr. Yasser Raoui
(Centre International d'Oncologie, AKDITAL EL JADIDA)

Speaker

Dr. Yasser Raoui is a medical physicist specializing in advanced radiation therapy and clinical dosimetry, holding a PhD in Medical Physics from Mohammed V University in Rabat. He possesses solid technical expertise in utilizing medical linear accelerators and treatment planning systems (TPS), with a specific focus on Quality Assurance (QA) for complex delivery techniques like IMRT and VMAT. Dr. Raoui's research contributions are centered on the crucial areas of pre-treatment verification—notably for carcinoma breast using mono-isocentric VMAT and 2D detector arrays—and the detailed beam modeling of equipment like Elekta MLCs within commercial TPS. He is also actively involved in Monte Carlo simulation for brachytherapy dosimetry. Combining scientific rigor and innovative methods, he is dedicated to optimizing radiotherapy workflows and ensuring the highest standards of patient benefit and quality of care.

Title: L'Intelligence Artificielle au service de la Radiothérapie

Abstract: L'intelligence artificielle (IA) transforme profondément la radiothérapie moderne en introduisant des algorithmes capables d'analyser, d'apprendre et d'optimiser l'ensemble du processus thérapeutique. Les techniques d'apprentissage profond permettent une segmentation automatique des volumes tumoraux et des organes à risque, tandis que les modèles prédictifs assistent dans la planification dosimétrique et l'évaluation de la toxicité. L'intégration de réseaux de neurones convolutionnels et de systèmes de décision basés sur machine learning favorise une standardisation accrue et une réduction significative des incertitudes. Par ailleurs, l'IA ouvre la voie à la radiothérapie adaptative en temps réel, où les traitements sont ajustés en fonction des variations anatomiques et biologiques quotidiennes. Ces avancées technologiques promettent une radiothérapie plus précise, personnalisée et efficiente, redéfinissant ainsi les standards de la prise en charge oncologique.

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EL JADIDA 18-19 DECEMBER 2025



Dr. Nezha Mejjad

(National Centre for Nuclear Energy, Science and Technology, Morocco.)

Speaker

Dr. Nezha Mejjad is a Research Scientist in Geochemistry & Environment at the National Center for Energy, Sciences, and Nuclear Techniques in Rabat, Morocco. Her academic journey began at the Faculty of Sciences Ben M'sik (Earth Sciences) at the University of Hassan II Casablanca, where she earned her Bachelor's degree in 2011 and her Master's degree in Applied Geology in 2013. In November 2018, she successfully defended her Thesis on 'Geochemical and radiometric approaches for assessing the intensity and chronology of metal trace element and radionuclide contamination in the Oualidia lagoon - Morocco'. Her academic prowess was further recognized when she was awarded her second Master's in 2019 in Sustainable Blue Growth from the National Institute of Oceanography and Applied Geophysics - OGS & University of Trieste, Trieste, Italy. In 2021, Nezha received her 3rd Master's Degree in Open Innovation and Youth Entrepreneurship In The Mediterranean Agri-food Sector from CIHEAMBari & University of Bari, Italy. She has contributed extensively to the field by 50 papers in international journals and 10 chapters' book showcasing her expertise in pollution assessment over the years and studying human activity and environmental interactions. Nezha was recently appointed as member of the editorial board of Communications Earth & Environment (Nature), Academic editor of the Journal Plos One, and Editorial board member of BMC-Environment, and Environmental Discovery Journal (Springer Nature). Also Nezha is currently editing a book entitled "Nuclear-Based Approaches Application for Marine Pollution Assessment and Monitoring" to be published within the book series "Environmental Science and Engineering" Springer, and co-editing two others books on Geotraces, marine ecosystems and environment.

Title: Space Weather: Toward the Forecasting of Geomagnetic Storms

Abstract: Solar activity refers to all the changes occurring in the Sun's magnetic field and atmosphere. These variations result from internal solar processes, particularly the movement of plasma and magnetic fields within the Sun. Solar activity takes many forms, including solar flares, sunspots, coronal mass ejections, and the solar wind. When these phenomena occur, they disturb Earth's magnetic field (the magnetosphere), producing geomagnetic storms of varying intensities. In this conference, we will introduce a new discipline currently developing in Morocco, dedicated to the study of these phenomena and their interactions with our biosphere: space weather. We will focus specifically on the study of geomagnetic activity through the planetary Kp index under extreme event conditions (major and severe storms). During such extreme events, Earth's environment and our technologies—both in space and on the ground—are affected by geomagnetic disturbances. To mitigate potential risks to technology during these events, a statistical analysis was carried out using a large dataset of Kp index values to identify geomagnetically active days over the last five solar cycles (20th to 24th).The evolution of the monthly occurrence probabilities across these solar cycles shows that these probabilities are higher during certain months than others. A significant correlation between the Kp index and sunspot numbers will also be highlighted.

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Pr. Rachid Amrousse
(Univ. Chouaïb Doukkali,
El Jadida, Morocco)

Speaker

He obtained his Bachelor's degree in 2006 from University of Chouaib Doukkali, El Jadida, Morocco. He then pursued his studies at the University of Poitiers in France, where he earned his Master's degree in 2007. In 2010, Prof. Amrousse obtalned his PhD degree from the University of Poitiers, collaborating with both the French space agency (CNES) and the Air Liquide Society. His doctoral research was centered on the topic of "The ignition of cold hydrogen oxygen mixtures for satellite control reactions." Following his PhD, in 2011, he became a Research Associate at the Japan Aerospace Exploration Agency (JAXA), becoming the first foreign national to be recruited by JAXA. His research focuses on the development of high-energy materials and the exploration of catalysis as applied to space propulsion, encompassing areas such as thermal decomposition, combustion mechanisms, characterization, and stability. In 2016, Prof. Amrousse secured a competitive grant from the Japan Society for the Promotion of Science (JSPS) for a two-year project aimed at developing green propellant thrusters for reaction control systems, particularly for small satellites. During the same year, he also joined University of Chouaib Doukkali, El Jadida, Morocco, where he eventually attained the position of Associate Professor in 2020. Throughout his career, Prof. Amrousse has received numerous allowances and awards for his research endeavors. These accolades include the Poitou-Charentes Region's Allowance for his Master's degree, CNES's allowance for his PhD degree, recognition from the European Green Aerospace Propellant (GRASP) Project, acknowledgments from JAXA, and support from JSPS. He has authored over 60 peer-reviewed papers and proceedings and has delivered more than 80 presentations, including oral presentations, keynote speeches, and plenary lectures, all revolving around propellant-related topics. He is an active member of the Japan Explosives Society. Prof. Amrousse is also an avid contributor to academic journals, reviewing more than 25 papers annually for various journals related to catalysis and propulsion. He edited several special issues and co-edited recently a book titled recent advancements in green propulsion, published by Springer Nature in 2024 and two other books with IGI Global. His achievements have been recognized with awards for best presentations, but perhaps most notably, he was awarded the National Medal of Merit by King Mohammed VI of Morocco in 2016.

Title: Recent Advancements in Green Propulsion: Sustainability in Space

Abstract: The demand for sustainable and environmentally friendly propulsion systems has catalyzed significant advancements in green propulsion technologies. This collection of book chapters offers a comprehensive overview of contemporary research and development efforts aimed at replacing conventional propellants with eco-friendly alternatives while maintaining or enhancing performance, reliability, and safety standards. The introductory chapter, "An Overview of Green Propellant and Propulsion System Applications: Merits and Demerits," provides a balanced perspective on the benefits and limitations of green propellants, highlighting their potential to revolutionize propulsion systems while addressing associated technical challenges. Subsequent chapters delve into specialized topics, such as the "Thermal and Catalytic Decomposition of Hydroxylammonium Nitrate (HAN)-Based Propellant" and the exploration of "Low-Cost Catalysts for Hydrogen Peroxide (H2O2) Thermal Decomposition," emphasizing advancements in catalyst design to improve efficiency and reduce costs. The state-of-the-art in Green Monopropellants is presented, showcasing the progress in formulation and performance optimization. Key engineering aspects are addressed in "Feed and Pressurization Systems and Architectures for Green Chemical Micro-Propulsion," highlighting innovative system designs for miniaturized applications, and in "Mono- and Bipropellants Based on Nitrous Oxide and Fuels: State of the Art," which examines the viability of nitrous oxide as a dual-mode propellant. The synthesis of academic and industrial advancements is explored in "Recent Developments in Academia and Industry and a Special Focus on DLR's Activities," offering a snapshot of cutting- edge research and practical implementations. Notable breakthroughs include the development of Ceramic Oxide-Based Non-Deactivating Catalysts tailored for HAN monopropellant thrusters and the resurgence of Hydrogen Peroxide Propulsion: Past Uses and Future Perspectives. Finally, the chapter "Development of Mono- and Bi-Propellant Systems for Green Propulsion Applications" consolidates findings from prior sections, underscoring the synergy of scientific innovation and engineering prowess in achieving sustainable propulsion solutions. This compilation serves as a vital resource for researchers and engineers seeking to advance the state of green propulsion systems, laying a foundation for a cleaner and more sustainable aerospace future.

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Pr. Rajaa Sebihi
(Univ. Mohammed V, Rabat, Morocco)

Speaker

Rajaa Sebihi is a qualified Professor and Researcher in the Department of Physics, Faculty of Sciences, at Mohammed V University in Rabat, Morocco. She is affiliated with the High Energy Physics Laboratory - Modeling and Simulation (LPHE-MS). Her specialization lies in Medical Physics and Radiophysics, specifically within the fields of Nuclear Medicine and Medical Imaging.

Title : Radiation Exposure from Medical Procedures: Ask the Medical Physicist

Abstract: A medical physicist plays a crucial role in managing radiation safety and effectiveness for medical exposures by evaluating equipment, optimizing doses, ensuring quality assurance (QA) programs, and providing training to staff on radiation protection practices. They work to minimize radiation risk while ensuring accurate and safe diagnostic or therapeutic outcomes by calibrating equipment, calculating patient and staff doses, and implementing protocols for safe use of radiation. and contributing to the development of new techniques and software for imaging and therapy. They also play a vital role in training, investigating incidents, and ensuring regulatory compliance.



Pr. Fatima Ezzahra Ramadan
(Univ. Mohammed V, Rabat, Morocco)

Speaker

Dr. F. Z. Ramadan is a Professor at the Higher School of Technology (EST–Salé), Mohammed V University, Morocco. Her research primarily focuses on computational condensed matter and materials physics. She applies ab initio methods, notably DFT and many-body perturbation theory, to explore the electronic, optical, and thermoelectric behavior of advanced materials. Her work concentrates on low-dimensional and hybrid materials, including graphene, silicene, GeC, SiC hybrids, and quantum dots. Dr. Ramadan has authored and co-authored several high-impact publications investigating optoelectronic and thermoelectric phenomena. Furthermore, she actively contributes to the scientific community by organizing conferences, serving on scientific committees, and participating in national and international research collaborations in computational materials physics.

Title : Advanced Nanomaterials for Emerging Technologies: From Fundamental Insights to Applications

Abstract: Two-dimensional (2D) nanomaterials represent a rapidly growing class of materials with immense potential for technological applications, including optoelectronics, spintronics, and energy conversion. Their unique structural, electronic, and magnetic features can be tailored through functionalization, doping, and nanoscale engineering, enabling unprecedented control over their performance in devices. This presentation will provide a comprehensive overview of recent advances in 2D nanomaterials, highlighting strategies to bridge fundamental understanding and practical applications. Key themes include the design of materials with tunable electronic and optical behavior, the engineering of magnetic states for spintronic applications, and optimization of thermoelectric properties for energy harvesting. Emphasis will be placed on the transformative role of these materials in developing next-generation technologies, illustrating how theoretical insights can guide the realization of high-performance devices.

International Conference on Frontiers in Quantum Simulation, Applied Physics & Energy Innovation (ICQPEI 2025)

EL JADIDA 18-19 DECEMBER 2025



Pr. Abderrahim Maftouh
(Univ., Cadi Ayyad, Marrakech, Morocco.)

Speaker

Dr. Abderrahim Maftouh is an Associate Professor at the Faculty of Sciences Semlalia, Cadi Ayyad University (Marrakech, Morocco), and a member of the Materials, Energy and Environment Laboratory (LaMEE). His research focuses on water treatment and renewable energies, particularly within the Water–Energy–Hydrogen Nexus and the valorization of non-conventional water resources for sustainable freshwater and green hydrogen production. He has authored and co-authored several scientific articles and book chapters published by Elsevier and Springer, and serves as a reviewer for numerous peer-reviewed journals indexed in Web of Science and Scopus. His teaching covers physics, desalination technologies, energy efficiency, and energy management (ISO 50001). Dr. Maftouh's work aims to advance integrated water–energy–environmental solutions contributing to sustainable development in Morocco and across Africa.

Effect of Inlet Pressure on RO System Behavior for Sustainable Hydrogen Production

Abstract: Reverse Osmosis (RO) has established itself over the past decades as the most prominent technology for brackish and seawater desalination. However, the impact of inlet pressure on RO performance, particularly when integrated into sustainable hydrogen production systems, is still not fully elucidated. This study addresses this gap by experimentally examining how variations in feed water pressure influence key operational and thermodynamic parameters of the RO process. A pilot-scale RO unit was developed and tested under controlled operating conditions. The effects of increasing feed pressure were analyzed with respect to salinity reduction (TDS), permeate flow (Q), specific energy consumption (SEC), recovery ratio (Y), and salt rejection (TR). Initial water quality measurements confirmed elevated salinity levels, making the case study particularly relevant. The results revealed that inlet pressure has contrasting effects on system behavior: TDS and TR decreased linearly with increasing pressure, while Q, SEC, and Y exhibited positive linear correlations. For instance, an increase to 10 bar reduced TDS by 20%, while SEC and Y rose by 15% and 12%, respectively. A mathematical model developed in parallel reproduced the experimental trends with high accuracy, demonstrating the reliability of the approach. These insights underline the importance of pressure optimization in RO systems, not only for improving desalination efficiency but also for their effective integration into green hydrogen production frameworks, thereby contributing to more sustainable and resilient energy–water systems.



Dr. Zakaria Zarhri
(SECIHTI , Autonomous University of the State of Morelos, Mexico)

Speaker

Dr. Zakaryaa Zarhri is a materials scientist and researcher at the Universidad Autónoma del Estado de Morelos in Mexico, with national recognition. He works at the intersection of computational modelling, advanced functional materials (for spintronics, hydrogen storage, corrosion resistance), and sustainable technologies. His academic role includes graduate teaching, student mentoring and contribution to the institutional research agenda in engineering and environmental technologies.

Title : Effect of Grain Size in Sprayed TiO_2 Semiconductors on its optical properties

Abstract: This work explores the structural, optical, and electrical properties of TiO_2 thin films applied in dye-sensitized solar cells (DSSCs). The influence of grain size and film thickness on the material performance was analyzed using experimental techniques and theoretical calculations. To enhance conductivity and stability, TiO_2 was deposited on conductive substrates and combined with a gel electrolyte. The results show that both crystallite size and layer thickness significantly affect the efficiency and durability of the solar cells, highlighting TiO_2 as a promising material for low-cost and sustainable photovoltaic applications.

International Conference on Frontiers in Quantum Simulation, Applied Physics & Energy Innovation (ICQPEI 2025)

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Pr. Amine Jaouadi
(LyRIDS, ECE-Paris, Graduate School of Engineering, Paris, France)

Speaker

Amine Jaouadi is a physicist specializing in quantum mechanics. He currently holds an Associate Professor position in the LyRIDS laboratory at ECE Paris, School of Engineering. His core research focuses on cold atoms, particularly Bose–Einstein condensates (BECs), which he studies using analytical and numerical approaches. Additionally, Dr. Jaouadi is interested in nonlinear dynamics within open quantum systems. This work includes studying the effects of dissipation, decoherence, and environmentally induced phase transitions. His work further explores the applications of these phenomena in quantum information. This includes the manipulation of qubits in ultracold gas-based architectures, and investigating the role of solitons and topological states in information processing protocols.

Title: Controlling Soliton Dynamics in Bose–Einstein Condensates for Quantum Technologies

Abstract: The ability to control the generation and dynamics of solitons in Bose– Einstein condensates (BECs) opens new perspectives for quantum technologies and nonlinear matter-wave engineering. In this work, we present a theoretical and numerical study of soliton formation in BECs confined by optical traps with tunable geometries and external barrier potentials. By employing crossed Laguerre–Gaussian beams with varying azimuthal index ℓ, the trapping potential can be continuously tuned from harmonic-like ($\ell = 1$) to square-well–like forms for larger ℓ, enabling the exploration of distinct dynamical regimes while maintaining the same condensate volume. Our findings demonstrate that trap geometry and barrier symmetry are powerful tools for tailoring soliton stability, interactions, and collective dynamics, paving the way for controlled soliton engineering with potential applications in quantum sensing, and nonlinear quantum optics.



Pr. Abdallah Slaoui
(Umiv. Mohammed V, Rabat, Morocco)

Speaker

Abdallah Slaoui is a theoretical physicist specializing in Quantum Technologies and Mathematical Physics, serving as a professor of physics at the Faculty of Sciences, Mohammed V University in Rabat, Morocco. He earned his Ph.D. from Mohammed V University and subsequently completed a postdoctoral fellowship at the Centre of Physics and Mathematics (CPM). Prof. Slaoui is a prolific researcher, having authored and co-authored numerous scientific papers and actively presented his findings at national and international congresses. His expertise is recognized by his role as a reviewer for scientific manuscripts submitted to many prestigious journals. Beyond his academic work, Prof. Slaoui is a member of the National Network of Young Researchers in Sciences and is passionately involved in both public engagement in quantum physics and the organization of national and international events.

Title : Quantum Information: An Overview of Promises and Challenges

Abstract: The significant expected societal impact of quantum technologies urges us to proceed and innovate responsibly. At the heart of this field are quantum resource theories, which are among the most intriguing and popular topics, providing a mathematical framework to quantify useful quantum phenomena, develop new detection protocols, and determine the exact processes that maximize their practical use. In this talk, I will discuss the fundamental questions of quantum resources in quantum information theory, presenting our most recent work that includes the characterization and quantification of entanglement and quantum correlations, as well as their role in quantum thermodynamics and quantum communication. Furthermore, we will discuss the importance of these resources in quantum metrology for surpassing the limitations of classical parameter estimation.

International Conference on Frontiers in Quantum Simulation, Applied Physics & Energy Innovation (ICQPEI 2025)

EL JADIDA 18-19 DECEMBER 2025



Pr. Brahim Amghar
(Univ. Chouaïb Doukkali,
El Jadida, Morocco)

Speaker

Brahim Amghar is an Assistant Professor of Theoretical Physics at the Faculty of Sciences, Chouaïb Doukkali University in El Jadida. He earned a Master's degree in Quantum Information and Cryptography and holds a Ph.D. in Mathematical Physics from the Faculty of Sciences, Mohammed V University in Rabat. His research explores the geometric and dynamical aspects of quantum correlations.

Title: Geometric Formulation of Quantum Information: From Hilbert Space to Quantum Phase Space

Abstract: We present a comprehensive geometric formulation of quantum information that builds a bridge between the abstract Hilbert space representation of quantum states and their description in quantum phase space. Starting from the Fubini–Study metric, we analyze how distances, angles, and geodesics capture fundamental quantum features such as entanglement, coherence, and state distinguishability. The geometric phase is then reinterpreted as a holonomic property of the underlying curved manifold, offering insights into its role in quantum computation and communication. We further explore the transition from Hilbert space to phase space via quasiprobability distributions, highlighting how symplectic structures provide an intuitive picture of quantum dynamics. This dual perspective reveals deep connections between quantum speed limits, brachistochrone problems, and the geometry of state space. By integrating entanglement measures with Riemannian curvature and phase space representations, our approach unifies geometric and informational aspects of quantum theory. This formulation not only clarifies foundational concepts but also suggests novel tools for optimizing quantum protocols and understanding the interplay between geometry, dynamics, and information processing.



Dr. Zakaria Mzaouali
(University of Tübingen
in Germany)

Speaker

Zakaria Mzaouali is a researcher at the University of Tübingen in Germany. He received his PhD at the Mohammed V University in Rabat, Morocco, for a set of work on correlations and work statistics in quantum many body systems. He started his quantum computing journey with a postdoc at the Institute of Theoretical and Applied Informatics, Polish Academy of Sciences. Currently, he works on characterization and benchmarking of quantum computers using the theory of quantum thermodynamics and machine learning.

Title : Quantum simulation on near-term quantum computers

Abstract: Quantum simulation seeks to reproduce the behavior of complex physical and chemical systems using controllable quantum hardware. This talk offers a clear, general overview of what near-term devices can achieve today. I will compare two leading approaches: D-Wave's annealing systems, which naturally search for low-energy configurations, and IBM Quantum's gate-based processors, which implement programmable sequences of quantum operations. Using illustrative examples from materials, chemistry, and optimization, I will show how these machines can provide insight despite real-world limits such as noise, calibration drift, and modest device sizes. I will also discuss practical, hybrid workflows that combine classical and quantum computing to make results more robust. I'll conclude with the role of AI—how learning methods can help choose problem encodings, tune control parameters, streamline experiments, and interpret noisy outputs—accelerating progress toward useful quantum simulation in the near term.

International Conference on Frontiers in Quantum Simulation, Applied Physics & Energy Innovation (ICQPEI 2025)

EL JADIDA 18-19 DECEMBER 2025



Dr. Sanae Samsam
(National institute of Nuclear physics, Milan, Italy)

Speaker

Sanae is an accelerator physicist at the Istituto Nazionale di Fisica Nucleare (INFN) in Milan, Italy. She earned her Ph.D. in Accelerator Physics from La Sapienza University of Rome in 2023, focusing on beam breakup and high-order mode instabilities in energy recovery linacs (ERLs). She holds a Master's degree in Quantum Physics from Mohammed V University in Rabat, Morocco, where she specialized in the simulation and modeling of pulsed and continuous fiber lasers. She also obtained two bachelor's degrees from the same institution, one in Mechanical Energy and another specialized in Medical Dosimetry. Her research interests include beam physics, inverse Compton scattering, and the development of compact light sources. She has played a key role in optimizing and simulating X-ray Compton radiation spectra for the STAR2 high-energy beamline, as well as high-order mode simulations for the BriXSinO project. She has also contributed to theoretical and numerical studies on a new regime called full inverse Compton scattering (FICS), exploring the possibility of complete energy and momentum transfer between electrons and photons. Sanae is deeply involved in the international accelerator community, having completed research stays at the Accelerator Test Facility (ATF) at Brookhaven National Laboratory, where she gained hands-on experience with high-brightness electron beams and laser-beam interactions. She is an active member of the International Organizing Committee (IOC) of the African Conference of Physics (ACP) and serves as a convener for the Accelerator and Compact Light Source working groups of ASFAP. She is also a member of the Executive Committee of the African Light Source (AfLS), contributing to strategic initiatives for synchrotron light sources in Africa.

Title : Advancing Science in Morocco with Compact Light Sources

Abstract: Accelerator-based light sources have become indispensable tools for advancing medicine, industry, cultural heritage, and fundamental research. Yet Africa remains underrepresented in this transformative field. Compact Light Sources (CLS), relying on Inverse Compton Scattering mechanism, offer a practical and cost-effective opportunity to bridge this gap. With moderate investment (≈ $10M), a CLS can be hosted on a university campus or a hospital, delivering high-brightness, tunable X-rays (5–300 keV) for applications in medical imaging, biophysics, and materials science, with upgrade potential to 500 MeV electron beams. Drawing inspiration from European examples such as Italy's STAR infrastructure, this talk outlines a proposal to establish a CLS in Morocco through national initiatives and international collaborations. Such a facility would strengthen scientific capacity, retain talent, and position Morocco as a regional hub within a Pan-African and Euro-Mediterranean research network. This initiative is envisioned as a strategic step toward the long-term goal of building the African Light Source.

Selected Oral Presentations

Conception and Characterization of Multifunctional Nanopolymer Coatings for Optimizing Photovoltaic Conversion Efficiency

Gouztal Oumaima[1], Younes Chrafih[1,2], and Mustapha Rouchdi[3]

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[3] Materials Physics Laboratory, Mohammed V University, Faculty of Sciences, Rabat, Morocco.

Abstract

This study examines the expansion of the solar photovoltaic (PV) sector under dual-carbon goals. Dust deposition and light reflection at the air-surface interface lower PV module performance. To increase solar panel efficiency, the researchers created a self-cleaning, transmission-enhancing multifunctional coating using the sol-gel technique. The coating demonstrated superior anti-fogging performance and a superhydrophilic surface with a water contact angle of just 2.076°. It raised light transmittance by 5 in the visible spectrum (380-760 nm). Additionally, the coating passed tape adhesion and 8 H pencil hardness tests, demonstrating its mechanical durability for outdoor use. The coating showed excellent surface resistivity during surface resistance tests, greatly lowering dust adherence.

Unveiling Thermal Robustness of Quantum Resources in Graphene-Based Qubits

Zakaria Bouafia[1], and Mostafa Mansour[1]

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

Abstract

Solid-state systems have emerged as highly promising candidates for realizing qubits in quantum technologies. Among these systems, graphene stands out as an exceptional platform due to its remarkable electronic properties and long coherence times. This presentation focuses on investigating the quantum properties of graphene that make it particularly suitable for advancing solid-state quantum technologies. We will explore how various system parameters influence the quantum resources in graphene, with special attention given to intraparticle entanglement, discord-type correlations, and coherence. We will present our research findings regarding the utilization of these resources. To quantitatively assess these properties, we will employ several quantum measures, including concurrence, local quantum uncertainty, and the relative entropy of coherence. Through our comprehensive analysis, our objective is to identify adjustable control system parameters that can effectively preserve quantum correlations and enhance coherence at intermediate temperatures. By showcasing the controllability of quantum correlations and coherence in graphene-based systems, our work contributes to paving the way toward the realization of practical quantum technologies.

Ti3C2 MXene multilayers: A DFT study of physical properties

Mohammed Gounzari[1,2], Abdelhadi Kotri[1,2], Youssef Belkassmi[1,2], Hamza Imtki[1,2] , El Houssine Atmani[1,2], Nejma Fazouan[1,2], and Mustapha Madi[1,2]

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[2]LMPSAES, FST of Mohammedia, Hassan II University, Casablanca, Morocco

Abstract

In this study, we used density functional theory (DFT) to analyse the structural, electronic, optical and thermodynamic properties of Ti3C2 MXene multilayers. The optical response, ascertained through dielectric functions, absorption spectra, reflectivity, refractive index, and transmittance, exhibits discernible patterns in relation to thickness. Our findings demonstrate that the properties of these MXene multilayers make them well-suited to high-performance optoelectronic and photovoltaic applications.

Correlations in a quantum-gravitationally coupled masses

Mohammed Gounzari[1], Rachid Ahl Laamara[1,2], and Moahmmed El Falaki [3]

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[2]Centre of Physics and Mathematics, Faculty of Sciences, Mohammed V University in Rabat, Rabat, Morocco,
[3]Laboratory of Innovation in Science, Technology and Modeling, Faculty of Sciences, Chouaib Doukkali University, EL Jadida, Morocco

Abstract

This study investigates the thermal and magnetic field dependencies of quantum coherence, quantum negativity, Local Quantum Uncertainty ($\mathcal{LQU}$), and Local Quantum Fisher Information ($\mathcal{LQFI}$) in a quantum-gravitationally coupled masses. Quantum negativity exhibits distinct peak behavior with shifts in temperature and decreases in magnitude as the magnetic field strength increases, highlighting the influence of stronger fields on the optimal temperature range, while quantum coherence displays a peak that shifts to higher temperatures, with its value decreasing due to thermal effects. The analysis reveals that thermal effects reduce coherence but moderate the suppression caused by the magnetic field, particularly at higher temperatures, in addition the dependence of quantum negativity on magnetic field strength, gravitational parameter, and coupling strength shows non-monotonic behavior with respect to the magnetic field and a monotonic increase with the gravitational parameter and stronger magnetic coupling suppresses quantum negativity. Moreover, $\mathcal{LQU}$ and $\mathcal{LQFI}$ show significant dependence on temperature and energy gap the magnetic field strength, $\mathcal{LQU}$ demonstrates a peak with broadening and reduced sensitivity to variations in the energy gap at higher temperatures, and shows a peak at low magnetic field strengths and decays as the field increases, with the decay more pronounced at lower temperatures while $\mathcal{LQFI}$ exhibits a more pronounced sensitivity to the energy gap at lower temperatures, with decreasing sensitivity as the temperature rises and exhibits a greater sensitivity to the magnetic field at lower temperatures, with a peak at a specific magnetic field and more gradual decay at higher temperatures.

MD-based Analysis of the Structural and Vibrational Behavior of Ag_xNi_{100-x} Metallic Glasses (x = 60–80)

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[1]LS2ME Laboratory, Polydisciplinary Faculty of Khouribga, Sultan Moulay Slimane University of Beni Mellal, Khouribga, Morocco

Abstract

Metallic glasses are amorphous solids that differ from conventional metals and traditional glasses due to their disordered atomic arrangement at the atomic scale. They find applications in various fields such as aerospace, electronics, and automotive industries. With the advancement of computational methods, it has been demonstrated that these tools can predict the behavior of materials, including metallic glasses. In this work, we employed molecular dynamics simulations within the LAMMPS environment to investigate an Ag–Ni system designed to form a metallic glass. The simulations were carried out using the Embedded Atom Method (EAM). Structural and vibrational properties of Ag–Ni metallic glasses were examined for three compositions (Ag_xNi_{100-x}, with $x = 60, 70$, and 80). The atomic structure was analyzed using several techniques, including the radial distribution function $g(r)$, Voronoi tessellation analysis (VTA), and coordination number distribution (CN). Furthermore, the vibrational density of states (VDOS) for the different compositions was obtained after system relaxation. The results indicate that, during cooling, the system volume increases with the silver concentration. The most dominant polyhedron observed across all compositions is $\langle 0, 0, 12, 0\rangle$, whose fraction rises with increasing Ag content. In terms of vibrational density of states, the intensity decreases as the silver concentration increases.

First-Principles (DFT) Investigation of (Ge/Sn)-Mn Halide Double Perovskites for Spintronic, Optoelectronic, and Energy-Conversion Applications

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Abstract

In this study, we present a comprehensive first-principles investigation of the structural, electronic, magnetic, and optical properties of Mn-based halide double perovskites $Cs-2(Ge, Sn)MnX_8$ (X = F, Cl, Br, I) using density functional theory (DFT). Structural stability is analyzed through the Goldschmidt tolerance factor and phonon dispersion calculations, confirming the robustness of their cubic phases. Electronic and magnetic analyses performed within the generalized gradient approximation (GGA), GGA+U, and the modified Becke Johnson (mBJ) approach reveal that these compounds are ferromagnetic semiconductors with tunable band gaps. Under the Heyd Scuseria Ernzerhof (HSE) hybrid functional, they exhibit half-metallic ferromagnetism

characterized by full spin polarization and high Curie temperatures. Optical calculations further show that halogen substitution significantly enhances the light-absorption properties, underscoring their strong potential for high-efficiency energy-conversion and optoelectronic applications. Overall, our results highlight the close interplay between crystal structure and physical properties, demonstrating the high tunability and technological relevance of this class of double perovskites.

Monte Carlo Simulation of Magnetic Properties and Hysteresis Behavior in a Mixed-Spin (5/2, 1/2) Ising Model on a Bilayer Graphene-Like Lattice

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[2]Team of Theoretical Physics, Laboratory L.P.M.C., Department of Physics, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco

Abstract

In this paper, we used Monte Carlo simulation based on the Metropolis algorithm to study the magnetic and thermodynamic properties and hysteresis behavior of a mixed-spin $(5/2; 1/2)$ graphene bilayer. To do this, we examined the impacts of exchange couplings, longitudinal crystal field, external magnetic field and temperature on magnetization, magnetic susceptibility, internal energy, blocking temperature, hysteresis behavior and its hysteretic parameters, namely coercivity and remanence. Interesting physical results were obtained, such as the richness of saturation values of magnetizations in the ground state and multi-loop hysteresis behavior.

Riemannian manifolds of two-mode Gaussian states evolving under parametric conversion and amplification processes

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Abstract

We consider some geometrical aspects associated with the dynamics of two-mode Gaussian states evolv- ing under two different processes: parametric conversion and parametric amplification. The evolved Gaus- sian states are represented by points of four dimensional manifolds. We employ the Hilbert-Schmidt to mea- sure the distance between two Gaussian states and we determine the Riemannian metric in each case. This study provides a geometrical description of the evolution from separable to entangled two-mode Gaussian states. This allows a geometric description of their evolution under time-dependent parametric interactions. Parametric conversion and amplification are quintessential in the manipulation of quantum states, enabling the transformation and enhancement of their entanglement properties. In particular, we focus on the investigation of the evolution of the entanglement in Gaussian states from

purely geometric perspective offering insights how parametric processes impact the manifolds curvature in connection with the entanglement generation.

Monthly Forecasting of Photovoltaic Production in Rabat, Morocco, Using Artificial Intelligence

Salma Riad[1], Naoual Bekkioui [1], and Hamid Ez-Zahraouy[1]

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Abstract

With the accelerated development of renewable energies, optimizing production is becoming crucial. In this context, artificial neural networks (ANNs) have become essential tools for modeling and predicting the output of photovoltaic systems, as they efficiently estimate power even under varying climatic conditions. In this context, this study proposes the development of an ANN model to estimate the average monthly power output of a 0.325 kW photovoltaic module installed in Rabat, Morocco. The proposed model incorporates several input variables, including the site's latitude and longitude, the month of the year, the panel tilt angle (ranging from 0° to 90°), and the nominal photovoltaic power (P). The predicted power (Pp) constitutes the model's output variable, serving as a reference for evaluating its accuracy. Two ANN architectures were compared to identify the most efficient configuration: one with two hidden layers and the other with three. Training was performed using the Levenberg-Marquardt optimization algorithm, known for its rapid convergence and efficiency in nonlinear regression problems. The data used for training and model validation came from real-world measurements collected in the Rabat region, thus ensuring an accurate representation of local conditions. The results clearly demonstrate that the three hidden layers architecture offers superior performance, notably due a greater reduction in prediction error. This improvement is reflected in a particularly high coefficient of determination (R^2), attesting to the robustness and reliability of the proposed model. This work thus highlights the potential of ANNs for optimizing PV production forecasting and supporting energy planning.

Étude du radon dans les eaux souterraines et superficielles : analyse expérimentale et implications radiologiques

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Abstract

Cette étude a pour but d'estimer les niveaux de radon présents dans divers échantillons d'eau prélevés dans la province de Midelt et la région de Drâa-Tafilalet, en ayant recours aux détecteurs solides de traces nucléaires (SSNTD). Le radon (222Rn), issu de la désintégration du 238U via le 226Ra, est un gaz radioactif naturellement rencontré dans les roches, le sol, ainsi que dans les eaux souterraines et, dans certains cas, dans les eaux

de surface. Son ingestion ou son inhalation peut conduire à une exposition aux rayonnements ionisants, ce qui rend son évaluation indispensable pour la protection sanitaire. Deux campagnes de prélèvement ont été réalisées: la première en décembre 2024 avec 15 échantillons, suivie d'une seconde en juin 2024 totalisant 10 échantillons. Les résultats de la première série montrent des différences notables selon le type d'eau : les puits présentent les concentrations les plus élevées (4,24 Bq/L), les eaux de barrage des valeurs intermédiaires (1,91 Bq/L), tandis que les eaux de rivière affichent les teneurs les plus faibles (0,84 Bq/L). Ces écarts reflètent l'impact des caractéristiques hydrogéologiques, notamment l'isolement des aquifères et la durée de séjour de l'eau. Pour les échantillons S1 à S10, les concentrations en radon varient entre 0,31 et 2,24 Bq/L, et les doses efficaces annuelles associées s'étendent de 2,09 à 8,83 Sv/an, selon l'origine de l'eau (puits, rivières ou barrages). L'ensemble de ces valeurs demeure largement inférieur aux seuils de référence fixés par l'Organisation mondiale de la santé, soit 100 Bq/L pour l'eau potable et 100 Sv/an pour la dose annuelle liée à l'ingestion. Les analyses montrent que les eaux étudiées renferment des quantités très faibles de radon, conformes aux normes internationales. Les doses efficaces calculées indiquent que l'exposition au radon à travers la consommation de ces eaux ne représente pas un risque notable pour la population.

Gate-based Counterdiabatic Quantum computing

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Abstract

In this talk, I will discuss the used Gate-based counterdiabatic quantum computing to solve the real industriel optimization problems on current state-of-the art quantum devices to achieve a quantum advantegeous.

Atomistic insights into nanoindentation-induced deformation of 3C-SiC single crystal.

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Abstract

Using molecular dynamics (MD) simulations, we investigated the effect of temperature on the nanoscale deformation behavior and mechanical properties of single-crystal (3C) silicon carbide (3C-SiC) (010) plane under nanoindentation. The simulation results showed that the atomic displacement and stress increased with increasing temperature. Thus, the nucleation and propagation of dislocations in the main slip systems were promoted to intensify the plastic deformation of the 3C-SiC crystal. The formation and propagation of prismatic loops was discussed. It was found that the hardness and

Young's modulus decreased with increasing temperature. The increasing temperature also contributed to the enhancement of the local phase transition from zinc blende (B3) crystal structure to wurtzite (B4) crystal structure and very obvious amorphization in the indentation region. This work can enrich the atomic-level understanding of the effect of temperature on the mechanical response of monocrystalline 3C-SiC when subjected to external loads.

Generated multi-transparency windows, Fano resonances, and slow/fast light in an opto-magnomechanical system with a mechanical membrane

M'bark Amghar[1], and Mohamed Amazioug[1]

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Abstract

This study presents a theoretical investigation of magnomechanically induced transparency, Fano resonances, and slow/fast-light phenomena within a a membrane-in-the-middle opto-magno-mechanical system. The system consists of a mechanical membrane inside a cavity and a ferrimagnetic crystal with a magnon mode that couples directly to a microwave cavity mode through magnetic dipole interactions and indirectly to an optical cavity via the crystal's deformation. The optical cavity is influenced by mechanical displacement driven by magnetostrictive forces through radiation pressure. Interactions among photons, phonons, magnons, and microwaves within the cavity give rise to optomechanically induced transparency (OMIT), magnomechanically induced transparency (MMIT), and magnon-induced transparency (MIT). We analyze the effects of opto-mechanical couplings on the absorption properties of the optical spectrum. Additionally, we provide an explicit explanation of the mechanism underlying the Fano resonance phenomenon. Moreover, we discuss slow light propagation: by tuning the opto-mechanical couplings, we achieve an enhancement of the slow light effect. Our results aim to contribute to the development of quantum information processing technologies.

New laser-driven effects in scattering and decay beyond the Standard Model

Mohamed Ouhammou[1], M. Ouali[1], S. Taj[1], and B. Manaut[1]

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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 Z0 , and laser-induced decay processes such as the decay of the proton into neutron, positron and electron neutrino.

Design of reactor for biogas and hydrogen production from organic waste mixed

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Abstract

This review explores recent advances in reactor for the co-production of methane and hydrogen from mixed organic wastes, focusing on the design and optimization of micro-methanizer systems. Using a systematic approach based on PRISMA-ScR, publications from 2022–2025 were retrieved from Scopus and Web of Science through targeted Boolean queries. Selected studies were analyzed according to reactor configuration, operational parameters, and modeling strategy. Results reveal that innovations such as bioelectrochemical enhancement, biochar-assisted digestion, and hybrid two-stage reactors significantly improve substrate conversion efficiency, microbial stability, and energy recovery. The review also discusses the application of ADM1-based models and control-oriented simulation tools for reactor performance prediction and scaling.Finally, it outlines current research challenges—including sensor integration, real-time monitoring, and reactor modularity—to guide the next generation of micro-methanizer design for sustainable bioenergy production.

Study of optoelectronic, thermoelectric and induced half-metallicity in Wurtzite ZnS via codoped (Eu, Cr): A DFT Method

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[5]Department of Physics, Mizoram University, Aizawl, 796004, India.

Abstract

Based on the Density Functional Theory (DFT), we have successfully examined the wurtzite sulfide (ZnS) codoped with the couple (Eu, Cr). This study generates the electronic, magnetic, optical, and thermoelectric (TE) properties by using the approach GGA and GGA+U. Our results find that the ferromagnetic alignment of spin is more stable than their antiferromagnetic coupling. Most notably, a half-metallic behavior

appears in the codoped material with 100 spin polarization at the Fermi level. However, the origins of ferromagnetism in the complex $Zn1-2xEuxCrxS, x = 0.0625$ is due to hybridization between S-3p, Cr-3d, and Eu-4f states in the case of the GGA approximation and p-f hybridization in the case of GGA+U. The insertion of double impurities leads to a compound with a large half-metallic gap. The optical simulation of ferromagnetism alloy reveals a high absorption coefficient at the ultraviolet spectrum level and a low reflectivity in the visible range. Furthermore, the calculation of the figure of merit ZT 1 proves that we have an efficient material for converting thermal energy into electricity. All these qualities combine to make $[Zn]_(1-2x)[Eu]_x[Cr]_xS$ a half-metallic ferromagnetism material efficient for spintronic, optoelectronic.

Dynamics of Quantum Correlations and Entanglement under Tunneling Asymmetry in Coupled Double Quantum Dot Systems

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Abstract

This paper investigates the impact of asymmetry in the tunneling energies on nonlocal correlations in a coupled double quantum dot system, using quantifiers such as concurrence, local quantum uncertainty, and Bell inequality violations. Concurrence and local quantum uncertainty help identify the optimal conditions for preserving entanglement and quantum coherence, while violations of Bell inequalities highlight the nonlocal nature of the states. The study shows that asymmetry enhances the preservation of correlations over time, while symmetry leads to faster dissipation but with more pronounced short-term oscillations. These findings emphasize the crucial role of asymmetry in maintaining quantum correlations and entanglement in situations that require temporal stability.

Parity symmetry breaking of spin-j coherent state superpositions in Gaussian noise channel.

Bouchra El Alaoui[1], Abdallah Slaoui [1,2], Abderrahim Lakhfif[1,2], and Rachid Ahl Laamara[2]

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[2]Centre of Physics and Mathematics, CPM, Faculty of Sciences, Mohammed V University in Rabat, Rabat, Morocco.

Abstract

The Wigner function and Wigner-Yanase skew information are connected through quantum coherence. States with high skew information often exhibit more pronounced

negative regions in their Wigner functions, indicative of quantum interference and non-classical behavior. Thus, the relationship between these two concepts is that states with high quantum coherence tend to display more non-classical features in their Wigner functions. By exploiting this relationship, which manifests as parity symmetry and asymmetry, we analyze parity symmetry and asymmetry in the superposition of two spin coherent states for a spin-1/2, as well as for a general spin-j. This analysis shows that the preservation of the parity asymmetry, or the violation of the parity symmetry, correlates with an increase in the value of spin j. Additionally, we investigate the behavior of parity symmetry and asymmetry of these states subjected to a Gaussian noise channel. Specifically, we examine how this parity symmetry and asymmetry change and identify the points at which parity symmetry is violated in the spin-1/2 cat state. Notably, the violation of parity symmetry becomes more pronounced at higher values of the decoherence parameter s. Our study shows how the spin value j affects the breaking of parity symmetry in general spin-j cat states that are hit by Gaussian noise.

A Convolutional Neural Network Approach for State of Charge Prediction of Batteries Using Time-Series Data

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Abstract

This work presents a detailed implementation of a Convolutional Neural Network (CNN) algorithm for predicting the State of Charge (SoC) of batteries using time-series data. The algorithm involves loading data from an Excel file, creating sequences for CNN input, normalizing the data, splitting it into training, validation, and test sets, defining the CNN architecture, setting training options, training the network, evaluating performance on validation and test sets, visualizing results, and saving the model for future predictions. The performance of the model is evaluated using metrics such as Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and the coefficient of determination (R^2). The training process completed in 151.56 seconds (2.53 minutes). The validation set performance showed an RMSE of 0.1722, an MAE of 0.1676, and an R^2 of -0.6345. The test set performance showed an RMSE of 0.1749%, an MAE of 0.1700%, an R^2 of -0.1021, and a maximum error of 0.3984%. The trained model is saved as `soc_cnn_model.mat` for future use.

Klein tunneling and Fabry–Pérot resonances in twisted bilayer graphene

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Abstract

We discuss the Klein tunneling and Fabry–Pérot resonances of charge carriers through a rectangular potential barrier in twisted bilayer graphene. Within the framework of the low-energy excitations, the transmission probability and the conductance are obtained

depending on the parameters of the problem. Owing to the moiré-induced anisotropy of the Hamiltonian in twisted bilayer graphene, the propagation of charge carriers exhibits an anisotropic behavior in Klein tunneling and Fabry–Pérot resonances. Moreover, we show that the anisotropy of the charge carriers induces asymmetry and deflection in the Fabry–Pérot resonances and Klein tunneling, and they are extremely sensitive to the height of the potential applied. Additionally, we found that the conductance is strongly sensitive to the barrier height but weakly sensitive to the barrier width. Therefore, it is possible to control the maxima and minima of the conductance of charge carriers in twisted bilayer graphene. With our results, we gain an in-depth understanding of tunneling properties in twisted bilayer graphene, which may help in the development and design of novel electronic nanodevices based on anisotropic 2D materials.

Magnetic PhaseTransitions and Hysteresis in Hexagonal Multi-layered Core/Double-Shell Nanowires

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Abstract

Weinvestigated the magnetic properties and phase transitions of a hexagonal Ising multi-layered core/double-shell nanowire comprising a spin-5/2 core, a spin-1 inner shell, and a spin-3/2 outer shell. Using Monte Carlo simulations based on the Metropolis algorithm and exact calculations of ground-state phase diagrams, we explored the system's behavior under various Hamiltonian parameters. The zero-temperature ground-state diagrams (GSDs) revealed multiple stable configurations with diverse topologies, including a compensation phenomenon for negative crystalline fields ( ). The phase diagram in the (T,) plane was mapped, identifying ferromagnetic, semi-ordered, and paramagnetic phases. The temperature dependence of total and partial magnetization was analyzed for different values of , external field (h), and interface exchange couplings (Jint). Additionally, hysteresis loops were studied under varying nanowire length (L), temperature (T), and Jint, revealing a strong correlation between these parameters and the loops' shape. This study provides significant insights for the design and optimization of next-generation nanomagnetic systems, with potential applications including, advanced memory storage devices and spintronic components.

Optically Controlled Topological Phases in the Deformed α–T_3 Lattice

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Abstract

Haldane's tight-binding model, which describes a Chern insulator in a two-dimensional hexagonal lattice, exhibits quantum Hall conductivity without an external magnetic

field. Here, we explore an α–T_3 lattice subjected to circularly polarized off-resonance light. This lattice, composed of two sublattices (A and B) and a central site (C) per unit cell, undergoes deformation by varying the hopping parameter γ_1 while keeping $\gamma_2 = \gamma_3 = \gamma$. Analytical expressions for quasi-energies in the first Brillouin zone reveal significant effects of symmetry breaking. Circularly polarized light lifts the degeneracy of Dirac points, shifting the cones from M. This deformation evolves with γ_1, breaking symmetry at $\gamma_1 = 2\gamma$, as observed in Berry curvature diagrams. In the standard case ($\gamma_1 = \gamma$), particle–hole and inversion symmetries are preserved for $\alpha = 0$ and $\alpha = 1$. The system transitions from a semi-metal to a Chern insulator, with band-specific Chern numbers: $C_2 = 1$, $C_1 = 0$, and $C_0 = -1$ for $\alpha < 1/2$, shifting to $C_2 = 2$, $C_1 = 0$, and $C_0 = -2$ when $\alpha \geq 1/2$. For $\gamma_1 > 2\gamma$, the system enters a trivial insulating phase. These transitions, confirmed via Wannier charge centers, are accompanied by a diminishing Hall conductivity. Our findings highlight tunable topological phases in α–T_3 lattices, driven by light and structural deformation, with promising implications for quantum materials.

Unlocking thermodynamic multitasking: Exploring the functioning of two-qubit engines through coherence and entanglement

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Abstract

Recent studies have investigated the role of entanglement in the operation of a two-qubit system as a heat engine, showing that work can be extracted from a single heat bath without direct heat dissipation between the two-qubit system and the cold bath (Bresque et al., 2021). In this work, we explore the impact of operating the same two-qubit system model with two heat baths and direct dissipation to the environment by applying both a local and a global Markovian master equation. The addition of a second heat bath enables the system to operate in different modes depending on the initial quantum state. We examine the temporal behavior of concurrence entanglement and quantum coherence, analyzing their observable roles in transitions between various operational regimes. Additionally, we investigate the evolution of information flow throughout the working cycle of the two-qubit system, focusing on the influence of individual and collective decoherence on the system's efficiency and operational modes. We identify the optimal parameter regions for the engine and refrigerator modes to achieve maximum performance. Finally, we investigate the effect of coherence outside the system on its thermodynamic quantities.

Investigation on novel two-dimensional TiB2P2 monolayer: A promising anode with high theoretical capacity for Li-ion batteries

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Abstract

The search for anode materials with significantly higher storage capacity remains a central challenge in the development of next-generation, high-performance lithium-ion batteries. Computational approaches, particularly those based on density functional theory (DFT), have become vital for accelerating the screening and rational design of candidate materials before experimental validation. In this context, we turned our attention to the two-dimensional TiB2P2 monolayer, a material that combines excellent structural stability with favorable electrochemical characteristics such as high theoretical capacity, low ion diffusion barriers, and good cycling performance. Its distinctive electronic structure, featuring Dirac cone states, further increases its appeal for fast charge transport. By evaluating the adsorption energies of lithium on various sites across the TiB2P2 surface, we identified the most energetically favorable positions for Li storage, revealing strong binding interactions that support efficient ion accommodation. Beyond adsorption behavior, the TiB2P2 monolayer demonstrates robust ionic and electronic conductivity, maintains a stable voltage profile during lithiation, and preserves structural integrity even under high Li concentrations. These properties collectively contribute to a substantial lithium storage capacity. Taken together, the combination of high stability, rapid ion mobility, and strong adsorption capability underscores the potential of TiB2P2 as a highly competitive anode material for next-generation lithium-ion batteries.

Magnetocaloric Potential of Ising Core-Shell Systems for Application in Magnetic Refrigeration Technology

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Abstract

We investigated the ground-state diagrams, the magnetic and magnetocaloric properties of a 2D square lattice Ising core-shell system using Monte Carlo Simulations (MCS) under the Metropolis algorithm in order to assess its magnetocaloric potential for application in magnetic refrigeration technology. We started our study by investigating the exact ground-state phase diagrams linked to interfacial exchange, applied magnetic field and anisotropy parameters, the obtained diagrams have exhibited various topologies. Afterwards, we moved to assess the main magnetic and thermodynamic quantities, namely the total and partial temperature-dependent magnetizations, magnetic susceptibility, magnetic heat capacity, as well as magnetic entropy which allowed us to evaluate the changes of entropy during magnetization and demagnetization in order to measure the magnetocaloric effect (MCE) of our system. The obtained results show two types of magnetization curves which vary slightly with interfacial exchange parameter, as well as wide range of temperature where entropy change values

are maximum, which is an interesting phenomenon for MCE and, subsequently, for magnetic refrigeration.

Pressure-driven homogenization of lithium disilicate glasses

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Abstract

Lithium disilicate glasses and glass–ceramics are promising for biomedical devices and solidstate batteries, and they serve as model systems for nucleation and crystal growth. These glasses also undergo phase separation that shapes their nucleation and crystallization behavior, yet the atomistic mechanisms—and their dependence on pressure remain unclear. Here, we combine molecular dynamics simulations with experimental corroboration to probe the spatial heterogeneity of lithium disilicate glasses prepared under pressure. We find that heterogeneity decreases as the cooling pressure increases, becoming nearly absent at 30 GPa. This trend originates from the pressure-suppressed attraction among Li cations that otherwise promotes clustering channels. By linking pressure to the attenuation of Lidriven clustering, our results clarify the origin of heterogeneity and provide guidance for designing glass–ceramics with controlled crystallization.

Hydrogen Storage Performance of 2D Materials: A Theoretical Study

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Abstract

Two-dimensional (2D) materials have attracted significant attention as promising candidates for hydrogen storage due to their high surface area and tunable electronic properties. In this theoretical study, density functional theory (DFT) calculations with dispersion corrections (DFT-D2 and DFT-D3) are employed to investigate the hydrogen storage performance of NbS_2 and Zr_2CO_2 (MXene) systems. For NbS_2, yttrium (Y) decoration markedly enhances the hydrogen adsorption capability. The Y-decorated NbS_2 surface can adsorb up to 28 H_2 molecules (seven per Y atom), corresponding to a

gravimetric hydrogen storage capacity of 3.10 wt% and an average adsorption energy of −0.161 eV, with an estimated desorption temperature of 206.16 K. Similarly, for Zr_2CO_2, lithium (Li) decoration substantially improves the hydrogen storage behavior. The optimized $8Li@Zr_2CO_2$ structure can accommodate up to 16 H_2 molecules with adsorption energies ranging from −0.162 to −0.233 eV, yielding a storage capacity of 1.52 wt% and a desorption temperature of 234.15 K. Both systems demonstrate good structural stability and favorable adsorption–desorption characteristics, suggesting their potential for reversible hydrogen storage. Although their gravimetric capacities remain below the DOE target (5.5 wt%), these findings provide valuable insights into the role of metal decoration and surface modification in enhancing hydrogen storage performance in 2D materials.

Probing Quantum Nonlocality and Entanglement in Coupled Double Quantum Dots under an External Magnetic Field

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Abstract

Double quantum dot (DQD) systems are promising platforms for implementing quantum information and computing technologies. We investigate quantum correlations (QCs) in a coupled AlGaAs/GaAs DQD system under varying temperature, energy detuning, coupling strength, and external magnetic fields. Quantum correlations are quantified using uncertainty-induced nonlocality (UIN) and Bell-type nonlocality, while entanglement is measured via logarithmic negativity. The results show that QCs are strongly dependent on thermal and system parameters: low temperatures enhance correlations, whereas higher temperatures suppress them due to thermal decoherence. Magnetic fields crucially influence resonance conditions, with maximum QCs occurring at zero detuning between DQDs. Conversely, large detuning or excessive coupling reduces correlations. These findings provide insight into the interplay between entanglement, nonlocality, and control parameters in DQD systems, offering valuable guidance for the design of future quantum devices.

Exploring Reheating in a Tachyon Model with Updated ACT Constraints

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Abstract

In this work, we investigate the reheating phase following tachyon inflation. We derive analytical expressions for the reheating temperature and the number of e-folds during reheating, assuming a constant effective equation of state. A comprehensive numerical analysis is then conducted across a wide range of model parameters. By incorporating the latest observational constraints from the Atacama Cosmology Telescope (ACT), we reassess the viability of tachyon inflation with an exponential potential within this scenario.

Improved Photocatalytic Efficiency of Sr5Ta4O15 Perovskite Oxide via V Doping and Oxygen Defects

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Abstract

Photocatalytic water splitting has emerged as a key approach to sustainable hydrogen production, yet many photocatalysts suffer from limited solar absorption and low conversion efficiency. In this study, we investigate the electronic, optical, and photocatalytic characteristics of $Sr_5Ta_4O_{15}$ through density functional theory (DFT) calculations, utilizing the generalized gradient approximation (GGA) for the exchange–correlation potential. The findings show that $Sr_5Ta_4O_{15}$ primarily absorbs ultraviolet (UV) light, which limits its photocatalytic activity to the UV range. To enhance its photocatalytic performance, we explore vanadium (V) doping in tantalum (Ta) sites and the introduction of oxygen vacancies (OVs). The results demonstrate a significant improvement in photocatalytic performance, with hydrogen production rates increasing from 2.18 μmol/g for pure $Sr_5Ta_4O_{15}$ to 259.8 μmol/g for V-doped $Sr_5Ta_4O_{15}$ with oxygen defects. Furthermore, the quantum efficiency (QE) and solar-to-hydrogen (STH) conversion efficiency improve notably, with the STH efficiency reaching 17.1%. These modifications help overcome light-harvesting limitations and contribute valuable insights toward the development of more effective photocatalysts for solar-driven hydrogen production.

Limits on the Reheating Epoch in Induced-Gravity Scenarios with a Holographic Description

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Abstract

In this work, we study an induced-gravity inflation model within a holographic framework, focusing on reheating driven by a quadratic potential. Although reheating is not directly observable, its key parameters—the temperature $T_{\rm re}$, the number of e-folds $N_{\rm re}$, and the effective equation-of-state $\omega_{\rm re}$—can be constrained by following the evolution of CMB modes from horizon exit to the present. Using the combined P-ACT-LB-BK18 dataset (ACT DR6, Planck 2018, BICEP/Keck 2018, and DESI), we derive updated bounds on the braneworld inflation scenario. We then explore how holographic effects and induced-gravity corrections influence these bounds, considering fixed $\omega_{\rm re}$ in the interval $-1/3 < \omega_{\rm re} < 1/3$. For parameter choices $c \leq 4 \times 10^7$, the model remains compatible with current observations, yielding a reheating duration consistent with the central spectral-index value and satisfying the lower limit on the reheating temperature.

Solar-Powered Airlift Reactor for Sustainable Landfill Leachate Treatment: Experimental Assessment and Contaminant Removal Efficiency

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Abstract

Landfills, characterized by their inherently challenging environmental impact, pose a significant threat to ecosystems. Uncontrolled waste disposal in landfills contributes to severe environmental issues, resulting in soil and water pollution. Addressing these challenges requires the development of novel and effective tools to mitigate the pollutant load associated with landfill sites. In this experimental study, we present a solar-powered airlift reactor with a specified effective volume (30 L) and equipped with stainless-steel electrodes. This forward-thinking design offers a sustainable alternative to conventional methods for managing landfill sites, marking a pioneering effort in adopting eco-friendly approaches. Furthermore, building upon the experimental results, this study critically examines the appropriate assumptions and experimental methodologies for applying adsorption isotherm models in the context of landfill management. The investigation delves into the removal rates of various contaminants, including chemical oxygen demand (COD), ammonia nitrogen (NH4+-N), phosphate (PO43–P), color, UV254, and metals. A comprehensive analysis of these parameters provides valuable insights into the efficiency of the proposed solar-powered airlift reactor system in mitigating the diverse pollutants associated with landfills.

Energy and Environmental Optimization of Educational Buildings Using Local Bio-Based Insulation

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Abstract

The purpose of this paper is to examine the effect of date palm fiber-based bio-insulation material on the energy and environmental performance of educational buildings in Meknes (Morocco). A multi-objective optimization was performed to minimize energy consumption, life-cycle cost, and CO_2 emissions, with simultaneous consideration for acceptable indoor thermal comfort. Optimization was carried out using the NSGA-II genetic algorithm combined with dynamic thermal simulations in TRNSYS, producing a Pareto front of optimal design solutions. Results show that both the thickness and the position of the insulation layer are crucial for achieving high performance. The use of date palm fiber as an insulation material decreases annual energy consumption by 47%, significantly reducing environmental impact. These findings highlight the potential of local bio-based materials to support sustainable and low-cost building design adapted to the Moroccan climate.

Lung Cancer Classification using Machine Learning and Data Augmentation

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Abstract

The classification problem is typically addressed using machine learning techniques. However, when there is an imbalance among classes in the data, these models often tend to overpredict the majority classes. As a result, the model exhibits low accuracy for some classes while achieving high accuracy for others. This challenge is particularly evident in lung cancer datasets, which contain 283 positive cases compared to only 38 negative cases. To mitigate this class imbalance, this study employs the Synthetic Minority Oversampling Technique (SMOTE), a well-known data preprocessing method. By comparing the performance of various machine learning models before and after applying this balancing technique, we identified Logistic Regression as the top-performing model, achieving an accuracy of 96.03% and a precision of 96.36%. Furthermore, after fine-tuning this model, we obtained an accuracy of 98.15%, an AUC of 99.92%, and a perfect precision of 100%. applications.

Enhancing AI-Based Breast Tumor classification by Integrating SPD-Conv into MobileNetV1

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Abstract

The accurate and dependable classification of breast tumors is of utmost importance for early diagnosis and effective treatment planning in clinical practice. Convolutional Neural Networks (CNNs) have been recognized as the dominant technology for medical image analysis, but their performance varies significantly across architectural designs. In addition, using heavy CNN architectures often requires cloud-based solutions, which raises concerns regarding patient-data privacy. Edge-based or embedded CNNs represent a more secure alternative, and MobileNetV1 is one of the most widely used architectures in resource-limited environments. However, its use of strided depthwise convolutions for downsampling often leads to a loss of fine-grained spatial information, which can significantly affect MobileNetV1 performance when recognizing breast tumors of varying sizes or when dealing with low-resolution breast imaging. In this work, we explore the integration of a Space-to-Depth Convolution (SPD-Conv) building block into MobileNetV1 to replace the strided depthwise convolution layers. SPD-Conv allows downsampling without discarding pixel-level details, thereby improving classification accuracy. We evaluate the SPD-augmented MobileNetV1 on a breast mammography dataset composed of a mix of INbreast, MIAS, and DDSM images, totaling 24,576 mass images (benign and malignant tumors). We observe an improvement of 1.62% in accuracy compared to the baseline model, reaching 92.06%, with a modest increase of approximately 2.1 million parameters. The proposed modification offers a balanced

trade-off between accuracy and model complexity, providing a lightweight and detail-preserving architecture well suited for embedded and edge-based tumor classification systems.

High Thermoelectric Conversion Efficiency in a Janus Silicon Oxy-Sulfide Monolayer: Insights from First-Principles Theory

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Abstract

In this study, we systematically investigate the electronic and thermal properties of the Janus silicon oxy-sulfide monolayer. Results based on density functional theory reveal that the monolayer is stable, exhibiting a tunable direct band gap and strong covalent bonding. Its ultralow lattice thermal conductivity (< 0.38 W/mK at 300 K) is attributed to the broken phonon selection rule for phonon–phonon scattering and a high level of anharmonicity, as reflected in the large Grüneisen parameter. Furthermore, the thermoelectric performance, assessed via the figure of merit, reaches 2.11 with a thermoelectric conversion efficiency of 15% for the n-type Janus SiOS monolayer, highlighting its potential for efficient waste-heat recovery applications.

First-Principles Insights into Double Perovskite Hydrides K2MgCoH6 and Rb2MgCoH6 for Next-Generation Hydrogen Storage

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Abstract

In this study, we used density functional theory (DFT) to analyse the structural, electronic, optical and thermodynamic properties of $Ti3C2$ MXene multilayers. The opticaUsing first-principles DFT calculations, this study looks at the possible use of two new double perovskite hydrides, K_2MgCoH_6 and Rb_2MgCoH_6, for storing hydrogen in solid form. Phonon dispersion and AIMD simulations confirmed the stability of the structure, making sure it would hold up in normal conditions. We examined the hydrogen storage capacity and desorption enthalpy. K_2MgCoH_6 performed better and had a lower H, which means it is more reversible. Elastic constants show that the material is mechanically stable, and the fact that the bulk moduli are relatively low suggests that hydrogen can move through it. Both materials have indirect wide band gaps, but K_2MgCoH_6 has stronger H-Co interactions. Thermodynamic parameters also show that these compounds can work well in real-world situations. In general, K_2MgCoH_6 is more stable and easier to store than Rb_2MgCoH_6, which makes it a better choice for hydrogen energy applications. response, ascertained through dielectric functions, absorption spectra, reflectivity, refractive index, and transmittance, exhibits discernible patterns in relation to thickness. Our findings demonstrate that the properties of these MXene multilayers make them well-suited to high-performance optoelectronic and photovoltaic applications.

Hydrogen Storage Potential of MBene Materials

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Abstract

Efficient and reversible hydrogen storage materials are essential to support the rapid growth of clean energy technologies. In this work, we examine the hydrogen storage capacity of lithium-decorated titanium diboride (TiB_2) monolayers as an MBene material. We conduct a systematic analysis of the structural stability, electronic properties, and hydrogen adsorption properties of pristine and lithium-decorated TiB_2 monolayers, using first-principles density functional theory (DFT) calculations combined with dispersion corrections. With strong binding energies (-3.38 eV), we observe that lithium atoms preferentially adsorb onto the most energetically favorable sites, effectively inducing charge transfer and polarization effects that enhance the interaction with hydrogen. With an adsorption energy of -0.20 eV/H_2, and both gravimetric and volumetric capacities of about 5.24 wt% and 95 g/L, respectively, in the $8H_2$@2Li@TiB_2 configuration, the optimized structures demonstrate the ability to adsorb multiple hydrogen molecules per lithium atom, thereby meeting the energy storage targets set by the U.S. Department of Energy (DOE).

Investigation of Vector-Like Top Quark Pair Production via $T \to H^+b$ Decays in Multi-b-Jet and Opposite-Sign Dilepton Final State at the LHC

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Abstract

We investigate the discovery prospects of a vector-like top partner (VLT) in the Type-II Two-Higgs-Doublet Model (2HDM-II) extended by a vector-like quark (VLQ) doublet (TB) at the 14 TeV Large Hadron Collider (LHC). In this work, the VLT is pair-produced via $pp \to T\bar{T}$ and predominantly decays through the cascade $T \to H^+b \to tbb$, with the top quark decaying leptonically. The resulting final state, comprising an opposite-sign lepton pair and multiple b-jets, offers a clean experimental signature. We evaluate the discovery significance as a function of the VLT and charged Higgs masses, integrated luminosity, and background systematic uncertainties. For $m_{H^\pm} = 600$ GeV and 5% systematic uncertainty, a 5σ discovery is achievable for $m_T \lesssim 1300$ GeV with 300 fb^{-1} luminosity. At higher luminosities of 1000 and 3000 fb^{-1}, the reach extends to 1500–1600 GeV, depending on the level of systematic uncertainty. While heavier $H^\pm$ masses reduce sensitivity, discovery remains attainable at high luminosity.

Clinical Evaluation of a Log-File–Based Quality Assurance System for IMRT and VMAT Treatment Delivery

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Abstract

The objective of this study was to evaluate the error detection sensitivity of a commercial log file-based system, LINACWatch® (LW), for potential integration into clinical routine, and to compare its performance with that of a measurement-based device, OCTAVIUS 4D (Oct4D), in the context of IMRT and VMAT delivery quality assurance (QA). A total of 76 treatment plans (head and neck, prostate, rectum, and breast) were analyzed after being preliminarily classified based on their Modulation Complexity Score (MCS), calculated by LW. Receiver Operating Characteristic (ROC) curves were used to establish appropriate gamma criteria for LW analysis. Twelve plans (three per treatment site) were intentionally modified to introduce delivery errors related to MLC, jaws, collimator, gantry, and monitor units (MU), resulting in 168 erroneous plans. These modified plans were irradiated and measured using Oct4D, while the corresponding log files were analyzed by LW. Each erroneous plan was compared to its error-free counterpart using gamma-index analysis for MLC, jaw, and MU errors, and root-mean-square (RMS) values for gantry and collimator errors. MCS values ranged from 0.10–0.20 for head and neck, 0.21–0.40 for prostate and rectum, and 0.41–1.00 for breast plans. Based on the ROC curves, the Gamma Passing Rate (GPR) thresholds were set at 87% for head and neck, 92% for prostate and rectum, and 99% for breast plans, using a 1.5%/1.5 mm/local gamma criterion. Results showed that LW demonstrated higher sensitivity in detecting the introduced errors compared to Oct4D, with detection rates of 48.5% and 30.4%, respectively. In conclusion, LW appears to be a valuable complement to phantom-based QA for IMRT/VMAT plan verification. The MCS tool proved effective in identifying under- or over-modulated plans prior to pre-treatment QA. Nevertheless, rigorous and routine machine quality controls remain essential.

Strain Effects on the Structural, Electronic, Optical, and Thermoelectric Properties of $SrTiO_3$

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Abstract

In this study, we used density functional theory (DFT) to analyse the structural, electronic, optical and thermodynamic properties of Ti3C2 MXene multilayers. The

optical response, ascertained through dielectric functions, absorption spectra, reflectivity, refractive index, and transmittance, exhibits discernible patterns in relation to thickness. Our findings demonstrate that the properties of these MXene multilayers make them well-suited to high-performance optoelectronic and photovoltaic applications.

Rare earth based scintillators for radiation detection

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Abstract

This study examines Rb2LuCl5 and Rb2PrCl5 through DFT analysis to assess their potential as rare earth based scintillators. Both compounds show dynamic stability from phonon results. Elastic data indicate higher isotropy in Rb2PrCl5 and stronger anisotropy in Rb2LuCl5. Electronic calculations reveal direct band gaps of 5.0698 eV for Rb2LuCl5 and 4.7022 eV for Rb2PrCl5. Optical properties show high transmittance and low reflectance at low photon energies. Predicted light yields reach 78898 photons per MeV for Rb2LuCl5 and 85066 photons per MeV for Rb2PrCl5. These results provide a clear view of the structural, electronic and optical behavior of two new rare earth based scintillation materials.

Structural, Electronic, and Optical Properties of $CuIn_{1-x}Ga_xSe_2$ Absorber Layers for Thin-Film Photovoltaics: A DFT+U and SCAPS-1D Study

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Abstract

This study employs density functional theory with Hubbard corrections (DFT+U) combined with SCAPS-1D device simulations to investigate the optoelectronic properties and photovoltaic performance of Ga-doped CuInGaSe (CIGS) semiconductors. Three compositions were examined: CuInSe (x = 0), CuIn.Ga.Se (x = 0.5), and CuGaSe (x = 1). DFT+U calculations reveal that gallium substitution systematically increases the direct bandgap from 1.04 eV to 1.68 eV at the point, while reducing lattice parameters from a = 5.788 Å to a = 5.619 Å. Electronic structure analysis shows the valence band maximum originates from Cu 3d–Se 4p hybridization, whereas the conduction band minimum derives from In/Ga s orbitals. Optical absorption coefficients enhance significantly with increasing Ga content, particularly in the visible spectrum. Device simulations using SCAPS-1D demonstrate that the optimal absorber layer thickness ranges between 1.0 and 2.0 m, with the intermediate composition (x = 0.5, Eg = 1.32 eV) exhibiting the highest power conversion efficiency.

Coupling Between Br-Hexahelicene Molecules Through Br···Br and Br···H Bonds

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Abstract

Non-covalent interactions, particularly halogen–halogen and halogen–hydrogen bonds, play a crucial role in the design of supramolecular and hierarchical nanostructures. This study investigates the intermolecular interactions that stabilize a dimer formed by two 2-Bromine-hexahelicen (Br-[6]H) molecules, which are chiral helical systems composed of six aromatic rings. Geometry optimization revealed two enantiomers, M and P, that can assemble into energetically equivalent homo-chiral dimers (MM and PP). Energy analysis shows that these dimers are stabilized by C–Br···Br–C (3.55 Å) bond, C–Br···H–C (2.97 Å) bonding, and van der Waals forces between molecules self-assembled. Using the Interaction Region Indicator (IRI), electrostatic potential mapping, and bond-path analysis, we clearly identify the interaction regions and confirm the presence of triangular Br···Br···H binding motifs. Overall, our results demonstrate the importance of halogen-halogen (X-X) bonding in developing functional molecular systems with potential applications in nanoscience, chiral materials engineering, and surface-based molecular devices.

Fabrication and Multiscale Characterization of a Biodegradable 3D-Printed Ferroelectret Designed for Mechanical Sensing

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Abstract

Ferroelectrets are cellular polymers exhibiting remarkable quasi-piezoelectric behaviour when charged under specified conditions (electric field, temperature, pressure, and environment). Ferroelectret have led to the development of various flexible sensors, actuators, and microenergy harvesters that are promising. Nevertheless, the majority of ferroelectrets are created using petrochemical-based materials that are non-biodegradable. Consequently, recycling such materials presents a significant challenge. This study presents a biodegradable 3D printed ferroelectret using Fused Deposition Modeling (FDM) that exihibit a closed and controlled cell geometry. It is an experimental approach that investigate the potential of three-dimensional printing in creating cellular polymers Polylactic acid (PLA) as a base for piezoelectric materials by focusing on the way the structural parameters affect the resultant porosity and electromechanical performance of the electret. The printed PLA have shown a good charge stability over 60 days with an interesting piezoelectric coefficient.

Modeling of Highly Efficient Lead-Free MASnI3-Based Solar Cell with Graphene Oxide as Hole Transport Layer Using SCAPS-1D

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Abstract

The remarkable electronic and optical properties of organic–inorganic halide perovskite materials have led to a significant increase in device performance. In this study, we used the SCAPS-1D numerical modeling tool to describe the optimized performance of a perovskite solar cell device based on methylammonium tin iodide ($MASnI_3$; MA = CH_3NH_3) using graphene oxide (GO) as the hole transport layer (HTL). Herein, different parameters impacting the efficiency of the solar cell are analyzed, including the thickness of both the $MASnI_3$ active layer and the GO layer, the defect density at the GO/$MASnI_3$ interface, the defects at the $MASnI_3$/ETL interface, the series resistance R_s and shunt resistance R_{SH}, and the operating temperature of the solar cell. The glass/FTO/ETL/$MASnI_3$/GO/Au structure was found to have optimal performance with an open-circuit voltage (V_{OC}) of 0.71 V, short-circuit current density (J_{SC}) of 34.83 mA cm^{-2}, fill factor (FF) of 77.59%, and power conversion efficiency (PCE) of 19.16%. These results demonstrate that by optimizing the device parameters, it is possible to experimentally obtain efficient lead-free perovskite solar cells.

Bidirectional Quantum Teleportation and Multi-Hop Quantum Networking: Protocol Design, Coherent-State Encodings, and Optimization via Quantum Walks and Algorithmic Techniques

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Abstract

This work presents a comprehensive framework for bidirectional quantum teleportation (BQT) and its integration into multi-hop quantum networking architectures. We develop a unified protocol that enables the simultaneous exchange of quantum states between distant nodes while accounting for network-level constraints such as routing, noise accumulation, and entanglement distribution. The information carriers are encoded in coherent-state superpositions, including even and odd Schrödinger-cat states,

enabling robust transmission in hybrid continuous-variable and discrete-variable settings. To optimize communication over large-scale quantum networks, we introduce a routing strategy based on discrete-time quantum walks combined with algorithmic techniques inspired by modified Dijkstra optimization, allowing the protocol to automatically identify high-fidelity paths across dynamically changing topologies. The full communication process—state preparation, entanglement generation, teleportation measurements, and recovery—is modeled using Kraus noise channels and evaluated through fidelity, quantum Fisher information, and Hilbert–Schmidt speed. We further validate the method through Qiskit and SimQN simulations on multi-node networks. Results show that the proposed BQT–MDQW protocol achieves improved fidelity, reduced entanglement loss, and shorter optimal paths compared to classical routing and unidirectional teleportation baselines. This study provides both a theoretical and computational foundation for scalable, high-performance quantum communication in next-generation quantum networks.

First-Principles Investigation of Structural Stability and Electronic Properties of TiS_2 Monolayer for Hydrogen Storage Applications

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Abstract

Two-dimensional TiS_2 has emerged as a promising material for solid-state hydrogen storage owing to its lightweight structure, large surface area, and tunable electronic properties. In this work, we employ density functional theory (DFT) to investigate the structural stability and electronic behavior of TiS_2 upon hydrogen adsorption. The calculations are performed using the GGA-PBE functional, including van der Waals corrections to account for weak interactions. The results indicate that TiS_2 maintains its structural integrity after hydrogen adsorption, while exhibiting a notable charge redistribution that promotes physisorption. These findings highlight TiS as a stable and efficient platform for reversible hydrogen storage, providing valuable theoretical insight into the design of advanced 2D energy materials.

Exploring LHC Constraints on Vector-Like Top Quarks within the 2HDM Framework

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Abstract

We investigate the phenomenological implications of extending the Two-Higgs-Doublet Model (2HDM) with vector-like top quarks (VLTs), emphasizing exotic decay channels

into non-standard Higgs bosons, T → Ht, T → At, and T → H+b, in addition to the conventional Standard Model (SM) modes. These beyond-the-SM (BSM) decays, currently absent from Large Hadron Collider (LHC) searches, can substantially alter the exclusion limits on VLT masses. In the Type-II 2HDM with a singlet VLT, the lower bound decreases from approximately 1.43 TeV to 1.28 TeV, while for a (T, B) doublet it drops from 1.54 TeV to 0.99 TeV, driven by the dominance of the T → H+b mode with a branching ratio approaching 98.

Surface dilution effects on the magnetic properties of ferrimagnetic core–shell nanomaterials.

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Abstract

Using Monte Carlo simulations (MCS), we investigated the magnetic properties and phase diagrams of a hexagonal ferrimagnetic Ising nanotube with a core–shell structure composed of spin-5/2 and spin-2 particles, taking surface dilution into account. Our results revealed several characteristic behaviors. Notably, the concentration of magnetic atoms has a signifcant infuence on both the critical and compensation temperatures. For low values of the exchange interaction Js, dilution has no efect on the critical temperature. However, a compensation point appears beyond a dilution threshold, observed for $x0.6$.We also identifed critical thresholds for the crystal feld anisotropies Ds and Dc. Below these thresholds, the critical temperature remains nearly constant, then gradually increases and converges toward a saturation value once the thresholds are exceeded. Furthermore, the analysis of hysteresis loops shows that the system's magnetic response is highly infuenced by dilution: the remanent magnetization increases signifcantly in absolute value as the concentration of magnetic atoms rises from 0.6 to 1.

Intégration of electronic didactic systems based on iot and automation to strengthen competencies in higher education

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Abstract

This research article analyzes the design, integration, and evaluation of didactic electronic systems based on IoT technologies and automation, implemented with the

purpose of strengthening technical and practical competencies in higher education students. A functional didactic module was developed integrating microcontrollers, sensors, actuators, wireless communication platforms, and real-time visualization tools. The study includes the characterization of electronic components, communication architecture, pedagogical system design, and experimental tests conducted in an academic environment. The results show significant improvements in the understanding of electronics, instrumentation, IoT networks, and automatic control concepts, as well as a notable increase in programming, analysis, and problem-solving skills.

Impact of Hidden Heavy Higgs Channels of VLB Quarks below 1 TeV in 2HDM

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Abstract

We investigate the impact of incorporating vector-like bottom (VLB) quarks into the Type-II Two-Higgs-Doublet Model (2HDM-II), introducing beyond-Standard-Model (BSM) decay channels $B \to Hb$ (CP-even), $B \to Ab$ (CP-odd), and $B \to H^- t$ (charged) that are distinct from Standard Model (SM) pathways ($B \to Zb$, $B \to hb$, $B \to Wt$). These BSM decays, currently unprobed by LHC searches focused on SM channels, significantly influence VLB mass constraints. In the 2HDM-II alignment limit with a singlet B, the VLB mass limit decreases from approximately 1.5 TeV to 1.32 TeV. For a doublet (T, B), the mass bound reduces from 1.55 TeV to 1.49 TeV. Notably, in the (B, Y) doublet configuration, the mass limit relaxes to below 0.98 TeV, driven by the dominance of $B \to Hb$ and $B \to Ab$ decays, whose combined branching ratios can approach 100%.

Magnetic properties and magnetocaloric effect of borophene monolayer doped : A Monte Carlo Study

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Abstract

The remarkable electronic and optical properties of organic–inorganic halide perovskite materials have led to a significant increase in device performance. In this study, we used

the SCAPS-1D numerical modeling tool to describe the optimized performance of a perovskite solar cell device based on methylammonium tin iodide ($MASnI_3$; MA = CH_3NH_3) using graphene oxide (GO) as the hole transport layer (HTL). Herein, different parameters impacting the efficiency of the solar cell are analyzed, including the thickness of both the $MASnI_3$ active layer and the GO layer, the defect density at the GO/$MASnI_3$ interface, the defects at the $MASnI_3$/ETL interface, the series resistance R_s and shunt resistance R_{SH}, and the operating temperature of the solar cell. The glass/FTO/ETL/$MASnI_3$/GO/Au structure was found to have optimal performance with an open-circuit voltage (V_{OC}) of 0.71 V, short-circuit current density (J_{SC}) of 34.83 mA cm^{-2}, fill factor (FF) of 77.59%, and power conversion efficiency (PCE) of 19.16%. These results demonstrate that by optimizing the device parameters, it is possible to experimentally obtain efficient lead-free perovskite solar cells.

Exploring Quantum Thermodynamics in MoS_2-Based Otto Engines under External Electromagnetic Control

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Abstract

we present a comprehensive study of an electromagnetically controlled MoS2-based quantum Otto cycle. By varying relevant physical parameters such as the initial and final momentum projections, electric field intensities, energy gaps, and system-reservoir couplings, we explore the complex thermodynamic behavior of the system. Special attention is given to identifying the operational regimes: engine, refrigerator, and accelerator, along with their respective thermodynamic efficiencies. This study provides insight into how the interplay between system parameters and external control fields governs the performance of the quantum Otto cycle. In particular, we demonstrate that fine-tuning the electromagnetic field can enhance efficiency, shift the boundaries between different regimes, and broaden the parameter space for robust engine operation. These results highlight the potential of MoS2 as a controllable platform for programmable quantum thermodynamic devices

Voronoi-Based Multi-UAV Deployement for Infrastructure inspection After Disasters

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Abstract

Following natural disasters, the rapid inspection of critical infrastructure is essential for ensuring public safety and guiding emergency response. To evaluate damage and

functionality, it is important to quickly assess key sites, such as hospitals, power plants, bridges, and emergency shelters. In this study, we propose an energyconstrained trajectory planning framework for a swarm of Unmanned Aerial Vehicles (UAVs) tasked with inspecting predefined infrastructure locations across a disaster-affected area. The approach begins by partitioning the affected surface using a Voronoi diagram and assigning each UAV a specific region to operate within. Within each region, the trajectory optimization problem is formulated as a mixedinteger linear programming problem (MILP) with an energy-based objective function. A genetic algorithm (GA) is applied to efficiently solve the optimization problem, and its performance is compared to the Nearest Neighbor Algorithm (NNA). The experimental results demonstrate that the GA achieves better energy consumption, whereas the NNA provides faster execution times.

Simultaneous Explanation of Light and Heavy Higgs Excesses in the N2HDM Framework

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Abstract

IRecent experimental hints from the Large Hadron Collider (LHC) in di-photon and partially in the $\tau^+\tau^-$ final states suggest the possible existence of an additional Higgs boson with a mass around 95 GeV. Interestingly, these observations are consistent with earlier results from the Large Electron-Positron (LEP) collider, which pointed to an excess in $b\bar{b}$ final states within a similar mass range. Additionally, CMS has observed an excess in the $\gamma\gamma b\bar{b}$ final state, indicating a possible resonance near 650 GeV decaying into a pair of SM-like Higgs bosons or into a SM-like Higgs boson accompanied by a lighter scalar with mass near 95 GeV. In this work, we investigate whether these anomalies can be simultaneously explained within the Next-to-2-Higgs-Doublet Model (N2HDM), an extension of the Standard Model (SM) scalar sector featuring two complex Higgs doublets and an additional real singlet. Assuming the existence of a CP-even Higgs state compatible with the 95 GeV excesses (restricted to the $\gamma\gamma$ and $b\bar{b}$ channels), we analyse the Type-II and Type-Y Yukawa structures, taking the observed 650 GeV resonance to be a CP-even Higgs state. An extensive parameter scan is performed, incorporating the latest constraints from the properties of the observed 125 GeV Higgs boson, direct searches for additional Higgs states, flavour physics data and Electroweak Precision Observables (EWPOs). Our results show that a heavy CP-even Higgs resonance around 650 GeV, produced predominantly via gluon-gluon fusion and subsequently decaying into a 125 GeV Higgs boson together with another scalar at approximately 95 GeV, can be simultaneously accommodated within both the N2HDM

Type-II and Type-Y frameworks at a significance level of 2σ. This interpretation leads to distinctive and testable predictions from the N2HDM for the ongoing LHC Run-3 and the forthcoming High-Luminosity LHC (HL-LHC) phase.

Systematic study of the dielectric and electrical properties of cesium doped potassium niobate KNbO3

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Abstract

Potassium niobate (KNbO3) is a functional material with highly interesting electrical and dielectric properties. In this experimental study, we investigated the influence of chemical composition on the dielectric characteristics ceramics. By varying the Cs/K ratio, we systematically measured dielectric permittivity and complex impedance over a broad frequency range. Our results demonstrate that the chemical composition has a significant impact on the dielectric properties of K1-xCsxNbO3. The observed variations are attributed to changes in the crystal structure and interactions between constituent ions. Moreover, we have highlighted a dielectric anisotropy linked to the preferential orientation of grains in the ceramics. This experimental study provides new insights into the underlying mechanisms of the dielectric properties of K1-xCsxNbO3 and opens up perspectives for the optimization of this material in various electronic applications.

TiNi thin film deposition on Ni substrates: A molecular dynamics analysis of incidence energy and temperature effects

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Abstract

TiNi thin film has become the most widely used shape memory (SMA) alloy in many industrial and medical applications. A thorough understanding of the growth mechanism is essential for achieving high-quality films. Experimental characterization techniques alone are insufficient to fully elucidate the growth mechanism at the nanoscale. Implementing advanced simulation techniques, such as molecular dynamics (MD), offers an effective solution to this issue. In this study, we investigated the atomic-scale growth of TiNi films using the MD method. The effects of the incident energy and substrate temperature are explored in details. The films deposited with an incidence energy of 0.1 eV show a rough morphology due to their low surface mobility. However, as the energy increased from 1 to 15 eV, the morphology became smoother.

This is explained by the high mobility of deposited atoms, which inhibits cluster formation on the surface [1]. Increasing the substrate temperature from 300 to 600 K slightly reduces the film roughness. This is due to the enhanced agitation of the atoms, which also promotes the filling of surface voids [2]. The results also show that at energies above 5 eV, at the film-substrate interface, some atoms from the film penetrate the upper layers of the substrate, while some atoms from the substrate are ejected into the film. The average atomic stress was calculated and found to be consistent with the experimental stress values. The stress increased with incidence energy, ranging from -105 to 270 MPa, and decreased with temperature above 500 K [3].

Approche géométrique de l'intrication dans un système bipartite de spins soumis à un champ magnétique externe

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Abstract

Cette étude explore les caractéristiques géométriques de l'intrication dans un système de deux spins du modèle XXX de Heisenberg soumis à un champ magnétique. Elle analyse l'évolution du système à travers la métrique de Fubini–Study, la vitesse d'évolution, la distance géodésique et la phase géométrique, tout en montrant l'influence du champ magnétique sur l'intrication.

Spintronic Investigation of Ferromagnetic Stability in Cr-Doped $Sr_{1-x}Cr_xX$ (X = S, Se, Te) Diluted Magnetic Semiconductors under Hubbard U Correction and Applied Strain

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Abstract

This study focuses on the electronic, magnetic, and elastic features of strontium chalcogenides SrX (X = S, Se, Te) doped with chromium (Cr) using ab-initio calculations, in the presence and absence of the Hubbard correction (U) and strain effect. The results show that adding Cr induces a half-metallic behavior and a stable ferromagnetic phase, with spin polarisation reaching 100 in the absolute majority of cases. The stability of this phase is confirmed by negative formation energies and high Curie temperatures, above room temperature, achieving its maximum values of 464K, 475 K, and 570 Kfor SrS, SrSe, and SrTe, respectively, at 24 of the chromium portion. The effect of applied strains (2and4) reveals a modulation of the electronic properties,

visualized by the shift in density of state (DOS) and the decrease of the band gap. A strengthening of the magnetic interactions while retaining the half-metallic character is also observed under strain. Since Cr-doped SrS has large elastic moduli and remarkable mechanical properties, it is a perfect choice for strong spintronic devices and spin filters that need mechanical stability. Its ability to blend mechanical strength and ductility makes Cr-doped SrSe a promising material for magnetic tunnel junctions (MTJs) in MRAM. For flexible spintronic devices, including SpinFETs, Cr-doped SrTe is an excellent choice due to its enhanced ductility (increased B /Gratio) and maximal deformability. These results highlight the potential of Cr-doped SrX compounds to improve device performance, efficiency, and functionality by relying on the interaction of ferromagnetism and elastic property tuning. The combination of all our findings makes our compound promising for spintronic applications

Characterizing non-Markovianity via quantum coherence

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Abstract

We present a new measure of non-Markovianity based on the property of nonincreasing quantum coherence via Kirkwood-Dirac (KD) quasiprobability under incoherent completely positive trace-preserving maps. Quantum coherence via the KD quasiprobability is defined as the imaginary part of the KD quasiprobability, which is maximized over all possible second bases and evaluated using an incoherent reference basis. A measure nonMarkovianity based on KD quasiprobability coherence would capture memory effects via the time evolution of the imaginary part of the KD quasiprobability, providing an experimentally accessible and physically intuitive alternative to traditional measures relying on quantum Fisher information or trace distance. This approach is applied to the study of dissipation and dephasing dynamics in single- and two-qubit systems. The results obtained show that, in the cases studied, our measure based on coherence via Kirkwood-Dirac quasiprobability performs at least as well as l1-norm coherence in detecting non-Markovianity, this provides a novel perspective on the analysis of non-Markovian dynamics.

Enhancing hydrogen storage performance of graphdiyne through high-vacancy defects and lithium functionalization: DFT study

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Abstract

One of the main obstacles to the advancement of hydrogen-based energy technologies is the creation of effective materials for hydrogen storage. In this study, we employ density

functional theory (DFT) with DFT-D3 corrections to investigate the hydrogen storage performance of graphdiyne sheet through high-vacancy defects and lithium functionalization ($Li8VGDY$). A 2×2 supercell of the graphdiyne monolayer was constructed by removing 30 carbon atoms and subsequently functionalized in-plan by eight lithium atoms. Ab initio molecular dynamics simulations at 300 K and the calculated negative cohesive energy reveal that Li_8VGDY is both thermally and thermodynamically stable. Furthermore, the calculated mean binding energy of functionalized Li atoms is significantly larger than the cohesive energy of bulk lithium. This indicates that lithium atoms remain dispersed on defected graphdiyne rather than forming metal clusters. Charge transfer analysis and electronic properties confirm significant electron donation from Li to the carbon framework, this situation renders Li atoms partially positively charged, which is favorable for adsorption of $H2$ molecules. For hydrogen storage performance, the system surpasses the U.S. DOE ultimate gravimetric target at 20 adsorbed H2 molecules, corresponding to 6.72 wt with an average adsorption energy of $-0.332eV/H2$ and a desorption temperature of 245 K. At highest capacity, the system achieves 21.92 wt with a mean adsorption energy of $-0.237eV/H2$ and a desorption temperature of 175 K, which lies within the optimal thermodynamic window for practical storage. These results highlight the synergistic effect of high-vacancy engineering and lithium functionalization in enhancing both the storage capacity and reversibility of graphdiyne for hydrogen storage.

Geometric Insight into Entanglement and Dynamics of Collective Spin Systems

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Abstract

With the growth of geometric science, including the methods of exploring the world of information by means of modern geometry, there has always been a mysterious and fascinating ambiguous link between geometric, topological and dynamical characteristics with quantum entanglement. Since geometry studies the interrelations between elements such as distance and curvature, it provides the information sciences with powerful structures that yield practically useful and understandable descriptions of integrable quantum systems. We explore here these structures in a physical system of N interaction spin-1/2 under all-range Ising model. By performing the system dynamics, we determine the Fubini-Study metric defining the relevant quantum state space. Applying Gaussian curvature within the scope of the Gauss-Bonnet theorem, we proved that the dynamics happens on a closed two-dimensional manifold having both a dumbbell shape structure and a spherical topology. The geometric and topological phases appearing during the system evolution processes are sufficiently discussed. Subsequently, we resolve the quantum brachistochrone problem by achieving the time-optimal evolution. By restricting the whole system to a two spin-1/2 system, we

investigate the relevant entanglement from two viewpoints; The first is of geometric nature and explores how the entanglement level affects derived geometric structures such as the Fubini-Study metric, the Gaussian curvature, and the geometric phase. The second is of dynamic nature and addresses the entanglement effect on the evolution speed and the related Fubini-Study distance. Further, depending on the degree of entanglement, we resolve the quantum brachistochrone problem.

Quantum sensing and metrology

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Abstract

Enhancing interferometric phase sensitivity is fundamental to advancing quantum sensing and precision metrology. We investigate the Mach–Zehnder interferometer under different phase-shift configurations and detection schemes, analyzing phase estimation through the quantum Fisher information and the quantum Cramér–Rao bound. Three detection strategies intensity-difference, single-mode intensity, and balanced homodyne are compared for their performance in single and two-parameter estimation. Our results show that with appropriately designed coherent input states, all detection schemes can achieve the ultimate quantum limit of phase sensitivity, demonstrating their potential for high-precision quantum measurements.

Achieving Optimal Multiparameter Quantum Estimation in Optomechanics

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Abstract

Accurate estimation of key physical parameters is essential for advancing the control and performance of optomechanical platforms. In this work, we study the simultaneous estimation of the effective detuning and the mechanical temperature T in a Fabry–Pérot cavity using quantum metrological tools. By deriving analytical expressions for the quantum Fisher information matrices associated with the symmetric (SLD) and right (RLD) logarithmic derivatives, we show that the RLD-based quantum Cramér–Rao bound consistently offers superior precision, particularly in non-commutative regimes. Our analysis reveals how optical power, cavity dissipation, and phonon and photon occupations influence the attainable sensitivity through their impact on quantum resources such as squeezing, purity, and optomechanical coupling strength. We further demonstrate that heterodyne detection can closely approach the ultimate precision allowed by quantum theory, making it a practical strategy for high-accuracy temperature estimation. These results provide valuable insights for optimizing optomechanical systems in quantum sensing and precision measurement applications.

High Thermoelectric Conversion Efficiency in a Janus Silicon Oxy-Sulfide Monolayer: Insights from First-Principles Theory

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Abstract

In this study, we systematically investigate the electronic and thermal properties of the Janus silicon oxy-sulfide monolayer. The results based on density functional theory reveal that the monolayer is stable. It exhibits a tunable direct band gap and strong covalent bonding. Its ultralow lattice thermal conductivity (<0.38 W/mK at 300 K), attributed to the broken phonon selection rule for phonon-phonon scattering and a high level of anharmonicity, as reflected in the large Grüneisen parameter. Furthermore, the thermoelectric performance, in terms of the figure of merit, is 2.11 with the thermoelectric conversion efficiency of 15 for the n-type Janus SiOS monolayer. highlighting its potential for efficient waste heat recovery applications.

Études des propriétés électroniques des matériaux 2D

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Abstract

DFTor density functional theory is a widely used quantum computing method, it is based on the idea that all the properties of a quantum system can be determined from its electronic density i.e. the spatial distribution of its electrons. indeed, this theory is used to study the electronic properties of materials, and in this regard, I have done studies on two materials which are silicon and graphene, this study contains: the convergence of the total energy and the cutoff energy, convergence of the total energy and the BZ(Kpoint) sampling, and the convergence of the total energy and the lattice parameter, in order to study the density of state and the band structure of the two materials.

Smart Solar Breakthrough: Machine Learning Powers Next-Gen CsSnI3/Si Tandem Cells

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Abstract

Tandem solar cells enhance the absorption of photons by utilizing materials that have different band gaps, allowing them to exceed the efficiency limits set by standard single-junction cells. In these configurations, the upper cell captures high-energy

photons, whereas lower-energy photons are transmitted to the lower cell for additional conversion. This research presents a computational study of a two-terminal tandem solar cell that merges a lead-free CsSnI3 top cell with a silicon bottom cell. The examination was carried out using SCAPS-1D simulations, which were improved with machine learning techniques to fine-tune device parameters like layer thickness and doping levels to achieve current matching and minimize losses from recombination. The CsSnI3 absorber was meticulously adjusted to improve charge carrier behavior and optimize optical absorption, while the silicon subcell was modeled based on the filtered light spectrum from the top cell. The optimized tandem configuration reached a PCE of 29.68, featuring a Voc of 1.675 V, a Jsc of 20. 47 mA/cm^2, and a FF of 86.53. These findings suggest the potential of machine learning-enhanced design in the development of high-efficiency, lead-free perovskite/silicon tandem solar cells. This methodology not only achieves impressive efficiency but also promotes sustainable and cost-effective photovoltaic technologies for future solar energy advancements.

Charging Efficiency and Correlation Effects in Double Quantum Dot Quantum Batteries

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Abstract

Quantum batteries (QBs) have been proposed as devices that take advantage of quantum resources, such as coherence and entanglement, to improve charge performance. This work presents a theoretical study of a quantum battery model based on two coupled double quantum dots (TDQDs) implemented on the AlGaAs/GaAs platform. Ergotropy and power are used as key indicators to analyze the influence of system parameters on energy performance. Results show that increasing the energy offset enhances ergotropy and power while reducing quantum coherence, whereas stronger tunneling couplings lead to a non-monotonic variation in ergotropy correlated with entanglement. These findings confirm the potential of quantum dots for efficient energy storage and emphasize that coherence alone is insufficient, with other quantum correlations being essential for optimal performance.

DFT study of functionalized graphyne quantum dot as pH-sensitive nanocarrier for berberine anticancer drug

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Abstract

To address berberine's low bioavailability and dose-limiting toxicity, we adsorbed it onto a hexagonal γ-Gy (γ-graphyne) quantum dot—also known as a graphyne spoked wheel—and analyzed the complex using density functional theory (DFT) calculations.

The calculated adsorption energy in the gas phase (−1.70 eV) confirms effective drug loading onto the nanocarrier. Thermodynamic parameters ($\Delta H = -2.18$ eV, $\Delta G = -1.36$ eV) indicate that the adsorption process is exothermic and spontaneous under physiological conditions. The negative adsorption energy in water further suggests that the berberine@γ-Gy complex remains stable during bloodstream circulation without premature release. Additionally, the increased dipole moments (up to 14.02 D) imply enhanced mobility and solubility of the drug–carrier hybrid. Frontier molecular orbitals (FMO), density of states (DOS), and partial DOS (PDOS) analyses reveal significant charge transfer from berberine to the graphyne quantum dot. Topological and noncovalent interaction analyses, including QTAIM, ELF, and NCI, demonstrate that a network of noncovalent interactions stabilizes the system and supports controlled drug release. Functionalization of the quantum dot with amine (NH_2) and carboxyl (COOH) groups introduces pH-sensitive behavior: strong binding is preserved at physiological pH, while a shift in adsorption energy to 2.32 eV under acidic tumor-like conditions enables targeted drug release. These findings highlight functionalized γ-graphyne as a promising pH-responsive nanocarrier for precision cancer drug delivery.
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Time fractional evolution of two dipolar-coupled spins under DM and KSEA interactions

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Abstract

is research investigates the time-fractional dynamics of two interacting dipolar spins in the presence of the Kaplan-Shekhtman-Entin-Wohlman-Aharony (KSEA) and Dzyaloshinsky-Moriya (DM) interactions, alongside a uniform external magnetic field. The main subject is to employ the time-fractional Schrödinger equation in order to examine the time-fractional development of quantum resources within the dipolar spin system, initially prepared in either a separable or partially entangled state. The study employs the norm of coherence, logarithmic negativity, and local quantum uncertainty to evaluate quantum coherence, entanglement and nonclassical correlations, respectively. This examination encompasses various parameters including the fractional derivative order, initial state configurations, strengths of DM and KSEA interactions, and dipolar coupling. Our main findings reveal that these quantifiers increase over time and evolve towards states of maximal coherence, regardless of whether the system is initially in a separable or partially entangled state. Lower values of the fractional derivative parameter are observed to enhance or steady the memory of the produced fractional state, which demonstrates the significant influence of fractional time dynamics. Additionally, strong DM and KSEA interactions significantly enhance the levels of

quantum correlations and coherence of the system, a trend mirrored by the dipolar coupling constants.

Bidirectional Quantum Teleportation through Noisy Channels via Multipartite Hybrid Entanglement

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Abstract

We propose and theoretically validate a bidirectional quantum teleportation protocol that enables two parties, Alice and Bob, to simultaneously exchange unknown quantum states with high fidelity through noisy dephasing channels. The protocol leverages a shared four-photon resource state with multipartite hybrid entanglement, where the polarization degrees of freedom are entangled with the frequency degrees of freedom, which act as a controllable environment. By engineering the initial system-environment correlations to precompensate for anticipated noise, the protocol effectively "hides" the quantum information from the decohering effects of the channel. We provide a rigorous mathematical framework for the protocol, including the initial state formalism, the dynamics under dephasing noise, and the state collapse following simultaneous Bell-state measurements. A critical finding is the necessity of cross-dependent unitary corrections, where each party's corrective operation depends on the measurement outcome of the other, requiring two-way classical communication. The protocol culminates in a "reverse decoherence" step, where the controlled application of further dephasing transforms the stored system-environment correlations back into coherence in the polarization subsystem, thus purifying the teleported states. Numerical simulations confirm the protocol's robustness, demonstrating that near-unity fidelity can be maintained for both teleported states even in the presence of significant channel noise, far surpassing the classical fidelity limit. This work extends the paradigm of noise-assisted quantum communication to bidirectional schemes, offering a more resource-efficient approach for robust information exchange in future quantum networks.

Approche géométrique de l'intrication dans un système bipartite de spins soumis à un champ magnétique externe

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Abstract

In this oral presentation, we present a unified geometric and dynamic framework for a two-spin system governed by Heisenberg's XXX Hamiltonian, with antisymmetric

Dzyaloshinskii-Moriya (DM) interaction and a longitudinal magnetic field. Using the Fubini-Study formalism, we calculate the quantum metric tensor and show that the system evolves on a compact three-dimensional torus whose geometric and topological structure captures the combined effects of spin-orbit coupling and magnetic anisotropy. We demonstrate that the geometric and topological phases accumulated along this toroidal manifold depend solely on the curvature and homotopy class of the trajectories, thus establishing a direct link between global topology and quantum coherence. Furthermore, we show that entanglement, quantified by Wootter's concurrence, modifies both the geometry and dynamics of the system: increasing entanglement increases the curvature of the manifold and accelerates its evolution, while DM interaction counteracts this by compressing the geometric structure and stabilizing the trajectories.

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Laser-induced optimization of entanglement and coherence in a two-qubit molybdenum disulfide system

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Abstract

In this work, we investigate the quantum information properties of a monolayer of molybdenum disulfide exposed to a polarized monochromatic electromagnetic field. Based on the density matrix at thermal equilibrium, we analyze both total and correlated quantum coherence (quantified by the l_1-norm), and thermal entanglement using concurrence. Our results show that, in the absence of external radiation, entanglement is favored at low temperatures and for small values of the band gap, spin-orbit coupling, and wave vector, but it rapidly disappears under the effect of thermal fluctuations, while coherence remains more robust. In the presence of a laser field, numerical results indicate that entanglement, although reduced in amplitude, becomes more resistant to temperature rise, while coherence is greatly amplified. This dynamic can be explained by photon-assisted transitions that renormalize the band structure and introduce new couplings between electronic states, partially stabilizing non-local correlations and reinforcing quantum superpositions. Finally, the strength, frequency, and polarization of the field are key control parameters, with circular polarization offering the most favorable conditions for simultaneously enhancing coherence and entanglement. These results highlight the dual role of electromagnetic radiation as a stabilizer and amplifier of quantum correlations, and confirm the potential of two-dimensional materials such as molybdenum disulfide for applications in quantum computing, secure communication, and high-precision detection.

Configurable Mach–Zehnder interferometer networks for distributed quantum sensing with squeezed-vacuum light.

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Abstract

We investigate a distributed quantum sensing protocol based on an array of d Mach–Zehnder interferometers (MZIs) for estimating relative phase shifts. The scheme employs d coherent states along with a single squeezed-vacuum state, which is distributed across the MZIs via a quantum circuit (QC). This protocol allows for analytical optimization, surpasses the shot-noise limit, and achieves the Heisenberg limit

with respect to the average total number of probe particles, n_T, for estimating arbitrary linear combinations of the d phases. We compare the entangled approach with a separable strategy that uses d coherent states and d squeezed-vacuum states under the same n_T. The entangled protocol significantly reduces resource overhead and can achieve a maximum gain of d when using the same total squeezed-light intensity as the separable scheme. Remarkably, employing a single squeezed-vacuum state in the entangled strategy can match the sensitivity of the separable approach that uses d copies of the state. Finally, for random QC configurations, we identify the optimal linear combination of phases that maximizes sensitivity. This approach opens the way to diverse applications in distributed quantum sensing with both photonic and atomic interferometers

Electronic, Thermodynamic, and Magnetic Properties of Cr and Mn (co)-doped cubic HfO2 for Spintronics Applications

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Abstract

This study focuses on analyzing the electronic, thermodynamic and magnetic properties of doped and co-doped 3D HfO2 materials using the Korringa-Kohn-Rostoker (KKR) Green's function method, combined with the coherent potential approximation (CPA) and the Generalized Gradient Approximation (GGA). Two types of impurities, chromium (Cr) and manganese (Mn), are examined. Density of states (DOS) calculations indicate that pure HfO2 is a semiconductor with a bandgap of 3.22 eV, while substituting Hf with Cr or Mn leads to metallic behavior. Initially, we discuss the equilibrium lattice parameter of HfO2. Subsequently, we study the band structure and DOS for both pure HfO2 and various dopant concentrations. The half-metallic (HM) character of the doped compounds is investigated, and the mechanism of exchange interaction is identified. In conclusion, by increasing the dopant and codopant concentrations, we successfully enhanced the Curie temperatures. These results are promising for spintronics applications, suggesting that doped HfO2 could be utilized in future spintronic devices.

Pressure-Induced Enhancement of the Photovoltaic Performance of the Lead-Free Double Perovskite Cs2NaScI6 : A DFT and SCAPS-1D Study

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Abstract

n this study, we investigate the pressure-dependent structural, electronic, mechanical, and optical properties of the lead-free halide double perovskite Cs2NaScI6 using density

functional theory (DFT) calculations and SCAPS-1D simulations. First-principles results reveal that the cubic phase of Cs2NaScI6 remains thermodynamically, mechanically, and dynamically stable under applied pressure. The reduction in band gap with increasing pressure enhances the optical absorption and charge carrier transport properties. Furthermore, the SCAPS-1D device simulation demonstrates an improved photovoltaic performance, achieving a power conversion efficiency (PCE) of about 19.31, confirming the potential of Cs2NaScI6 as a promising absorber for lead-free perovskite solar cells.

Numerical investigation of the Green Function Method to improve the effect of dot size on the photonic properties of InAs/GaAs Quantum Dots implemented in P-i-N Solar Cells Application

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Abstract

Quantum dot (QD) technology, based on the implementation of quantum dots in the intrinsic region, has attracted much attention because it takes advantage of photons with energies lower than the band gap for achieving high solar conversion efficiency. However, there is still a need for optimizing many parameters related to the solar cells, such as the nature of quantum dots and semiconductor materials. The main objective of this study is to enhance the impact of dot size on the photonic properties of InAs/GaAs Quantum dots in p-i-n solar cells (QDSC) applications through a numerical investigation using the Green Function Method. Our results show that open-circuit voltage weakly depends on dot size for both systems, while short-circuit current density is increased as dot size decreases. As a result, maximum efficiency values provide us with some guidance on the dot size on the photonic properties of InAs/GaAs Quantum dots to achieve better QDSC performance.

Study of Boron Neutron Capture Therapy (BNCT) Using Simulation with Geant4

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Abstract

Boron Neutron Capture Therapy (BNCT) is an innovative cancer treatment that selectively targets tumor cells enriched with boron-10 using thermal neutrons. This study investigates BNCT for brain tumors through Monte Carlo simulations with

Geant4, focusing on energy deposition in various cell compartments. Simulations demonstrate that BNCT delivers high doses to boron-containing tumor cells while sparing healthy tissues, highlighting its precision and potential clinical advantages. The choice of Physics Lists, including QGSP-BIC-HP, QGSP-BIC, and Geant4-DNA, significantly affects simulation accuracy. QGSP-BIC-HP proved particularly effective for modeling low-energy neutron interactions critical to BNCT, whereas Geant4-DNA provides detailed nanoscale insights. Results indicate higher energy deposition in the cell membrane compared to the nucleus, emphasizing the importance of Physics List selection based on research goals. Future improvements in boron delivery and neutron beam optimization are essential to enhance BNCT efficacy. These findings underline BNCT's transformative potential as a targeted alternative to conventional radiotherapy for aggressive brain tumors.

Critical Behavior and Magnetic Properties of Manganite-Derived Oxide La0.67Sr0.33MnO3

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Abstract

bstract The critical behavior and magnetic properties of La0.67Sr0.33MnO3 (LS33MO) have been studied using Monte Carlo simulations (MCS). Based on the Ising model with up to third-nearest-neighbor exchange inter- actions, we computed magnetic and magnetocaloric properties. The results show a Curie temperature (TC) close to the experimental value. The maximum magnetic entropy change (S max m) for an applied field of h = 5T is about 3.67 J K1kg1 , agreeing with experimental findings. The critical exponents were deter- mined to be = 0.306, = 1.178, and = 4.025, which were validated by the Widom scaling relation and universal scaling hypothesis

New perovskite hydride materials for hydrogen storage: DFT calculation

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Abstract

We examined physical properties of simple hydride perovskite materials, in order to show their potential for involving the storage of hydrogen. These investigations were conducted employing ab initio calculations based on density functional theory using the GGA-PBE and mBJ methods within the WIEN2k simulation code. Therefore, the structural optimizations of studied compounds exhibit stable cubic crystal structures. The electronic calculations reveal a consistent metallic behavior of all compounds.

Moreover, the analysis of storage properties show that the hydrogen storage properties of our materials show a great behavior, highlighting the importance of these new materials for hydrogen storage applications.

Perovskites for High-Performance Solar Energy Conversion

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Abstract

Perovskite materials are emerging as promising candidates for sustainable energy technologies owing to their remarkable optoelectronic characteristics. In this work, we employ density functional theory (DFT) to investigate the structural, electronic, optical, and photovoltaic properties of the chalcogenide perovskite $BaHfS_3$ in its stable orthorhombic phase. The compound exhibits a direct band gap and anisotropic carrier transport, characterized by low effective masses, high mobilities, and low exciton binding energies (22–45 meV), all of which contribute to efficient charge separation. $BaHfS_3$ also demonstrates a strong visible-light absorption coefficient of approximately 3×10^5 cm^{-1}, confirming its potential as an efficient energy-conversion material. Furthermore, device simulations performed using SCAPS-1D for an $FTO/ZnO/BaHfS_3/NiO_x/Ni$ architecture achieve a high power-conversion efficiency (PCE) of 23.65%, highlighting its promise for next-generation solar cell applications.

Novel Ti-doped Rb2BI6 (B = Zr or Hf) double perovskites for photovoltaic and photocatalytic applications: A first-principles study

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Abstract

Halide double perovskites have recently attracted significant attention for solar cell applications due to their enhanced power conversion efficiency, lower cost, and simplified fabrication. In this study, the structural, electronic, mechanical, and optical properties,

as well as the photocatalytic activity of Rb2BI6 (B= Zr or Hf) compounds, were systematically examined using first-principles calculations based on density functional theory (DFT). Using the PBEsol-GGA+mBJ approximation, the calculated band gap values were found to be 3.235 eV for Rb2ZrI6 and 4.163 eV for Rb2HfI6, which are in good agreement with experimental results. Furthermore, the compounds Rb2B1-xTixI6 (where B= Zr or Hf and x = 0.0, 0.25, 0.5, 0.75, and 1.0) exhibit p-type semiconducting behavior with direct band gaps. Upon substituting Zr and Hf atoms with titanium, the band gaps decreased from 2.983 eV (x = 0.0) to 1.802 eV (x = 1.0) for Rb2Zr1-xTixI6 and from 3.865 eV (x = 0.0) to 1.871 eV (x = 1.0) for Rb2Hf1-xTixI6, when spin–orbit coupling was taken into account. The decrease in band gap enhances visible light absorption, particularly when the compounds are fully doped with titanium (x = 1.0). Moreover, all studied compounds were found to be thermodynamically stable, as confirmed by their negative formation enthalpy values. Notably, the doped compounds demonstrated the potential to generate hydrogen via water splitting. These findings highlight that Rb2B1-xTixI6 (where B = Zr or Hf and x = 0.25, 0.5, 0.75, and 1.0) are promising p- type semiconductors for use in photocatalytic and photovoltaic applications.

Mechanical Enhancement of Cemented Radioactive Liquid Organic Waste Using Activated Bentonite as a Functional Additive

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Abstract

Radioactive organic wastes are produced as a result of nuclear fuel cycle operations, radioisotope production, and their use in medicine, research, and industry. In Morocco, the generated radioactive waste consists mainly of low- and intermediate-level waste, such as liquid organic waste (LOW). Cementitious materials are widely used in the nuclear industry for the conditioning and containment of such waste, including LOW. This study introduces a novel approach to enhance the mechanical performance of solidified waste formulations by incorporating activated bentonite. Three LOW dosages (16 wt%, 18 wt%, and 20 wt%) were evaluated. The mechanical properties—including compressive strength and porosity—were investigated using microstructural and mineralogical analyses. Results indicate that the incorporation of activated bentonite significantly improves compressive strength, reaching values above 14 MPa after 28 days of curing, with a 33% increase compared to previous formulations. Microstructural analysis reveals calcium silicate hydrate (C–S–H) as the main hydration product responsible for strength development. The incorporation of activated bentonite not only enhances mechanical stability but also reduces the final waste volume, offering an efficient and viable solution for the cementation of radioactive LOW.

Investigation of how the storage duration of spent radioactive ion exchange resins affects the quality of their conditioning through cementation.

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Abstract

Radioactive waste in Morocco is mainly generated by using radioactive materials in various sectors, such as health, industry, and agriculture. Spent radioactive ion exchange resin (RIE), the subject of this study, is considered a long-lived low- and medium-level radioactive waste. It is produced after its use for the purification of the water circuits of the TRIGA MARKII nuclear reactor at the National Center for Energy, Science and Nuclear Technology (CNESTEN-Morocco). The radioactive spent resin thus generated must be managed appropriately to minimize the potential risk to human health and the environment from exposure to ionizing radiation. The cementing conditioning process is the most widely used to contain this type of waste. Typically, spent RIE is collected and stored until it reaches the right volume to begin cementing. In this context, a study was carried out to comprehensively assess the impact of storage time on the quality of the cemented resin package. Several forms of waste cemented with RIE were produced. The RIE load assumed by the cementing formulation used is set at 14.38. The impact of the storage life of the spent RIE was assessed by monitoring and controlling the durability and mechanical performance of the RIE shapes produced.

Ab Initio Investigation of Spintronic Enhancement in Vanadium-Doped CaTiO3

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Abstract

The structural, electronic, and magnetic properties of vanadium-doped $CaTiO_3$ were investigated using *ab-initio* calculations to explore its potential for spintronic applications. For the undoped compound, an indirect band gap of 1.86 eV was obtained using the KKR–CPA–LDA method, confirming its semiconducting behavior. Depending on the vanadium concentration, the spin polarization at the Fermi level approaches

100%. The density of states analysis reveals features of both metallic and half-metallic behavior, while total energy calculations indicate that the ferromagnetic state is the most stable. Notably, at 8% V doping, the Curie temperature increases to 466 K, exceeding room temperature, which highlights the material's promise for future spintronic device applications.

Quantum Interferometric Power Versus Local Quantum Uncertainty in Bell Coherent States Under Amplitude Damping

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Abstract

Non-classical correlations, quantified by uncertainty measures such as Local Quantum Uncertainty (LQU) and Quantum Interferometric Power (QIP), are vital resources in quantum information, existing even in non-entangled mixed states. This study investigates the quantum correlations of Bell cat states under amplitude damping, employing LQU and QIP as quantifiers. This work investigates the dynamics of these correlations in two-mode Bell cat states under the influence of amplitude damping noise. We derive analytic expressions for both LQU and QIP for these states, which are constructed from Glauber coherent states. Furthermore, the study explores the potential of these correlations for enhancing phase estimation precision in quantum metrology. We also analyze the resilience of non-classical correlations, quantified by LQU, in Bell cat states subject to phase damping, depolarizing, and phase reversal channels. Our results provide crucial insights into the robustness and utility of these correlations, highlighting their significance for quantum information processing and communication.

DFT Study of the Effect of Ti, Ca, and Li Substitutions on the Hydrogen Storage Properties of ZrNiH

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Abstract

In this work, a computational investigation is carried out on the structural, thermodynamic, and electronic properties of substituted $ZrNiH_3$ hydrides for hydrogen storage applications. The ground-state geometries, formation energetics, and electronic structures of $Zr_{1-x}M_xNiH_3$ (M = Ti, Ca, Li) were systematically studied using Density Functional Theory (DFT) within the B3LYP framework. The influence of elemental substitution on lattice stability, metal–hydrogen interactions, and electronic density of states (DOS) is analyzed to clarify the relationship between atomic substitution and

hydrogen storage performance. Key parameters such as formation enthalpy (ΔH), hydrogen desorption tendency, DOS/PDOS characteristics, and modifications of the Zr–Ni–H bonding environment are calculated and discussed.
Understanding these thermodynamic and electronic descriptors is essential for the design of optimized metal hydrides. The results indicate that Ti, Ca, and Li substitutions can effectively tune the stability of $ZrNiH_3$, making the modified compounds promising candidates for enhanced hydrogen storage systems.

The LiBeH perovskite emerges as a promising candidate for efficient hydrogen storage.

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Abstract

Hydrogen storage is essential for the development of clean and efficient energy systems. In this work, the perovskite $LiBeH_3$ is investigated using density functional theory (DFT) to evaluate its structural, electronic, and hydrogen storage properties. LiBeH shows a high storage capacity (15.93 wt) and strong structural stability. Theoretical analyses, including formation energy, AIMD, Elastic constants, and phonon calculations, confirm its thermodynamic and mechanical stability. These results highlight LiBeH as a promising material for next-generation hydrogen storage applications.

GEANT4-Driven Simulation of Boron Neutron Capture Therapy (BNCT)

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Abstract

Cancer remains a major global health issue, with tumors such as glioblastoma presenting significant challenges for conventional treatments due to their infiltration into healthy tissue and high recurrence rates. Boron Neutron Capture Therapy (BNCT) is emerging as a promising solution, utilizing the nuclear properties of boron to selectively target cancer cells while sparing healthy tissue. Methods: BNCT involves administering a boron-containing drug followed by neutron irradiation, which triggers nuclear reactions that release high-energy particles, primarily damaging tumor cells. This study develops a simplified mathematical model of boron-loaded brain cells, structured into four compartments (nucleus, cytoplasm A, cytoplasm B, and cell membrane), to simulate energy transfer and predict treatment effectiveness. Simulations were conducted using GEANT4. Results: The model provides detailed insights into neutron-tissue interactions, highlighting areas for optimizing boron dosage and neutron delivery. Conclusion: The findings support improved BNCT strategies, with the potential to enhance treatment outcomes for aggressive tumors such as glioblastoma.

First-Principles Investigation of the Structural and Hydrogen Storage Properties of the Perovskite-Type Hydride $LiSiH_3$.

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Abstract

Hydrogen storage remains a key obstacle in the advancement of clean and sustainable energy technologies. In this work, first-principles calculations within the framework of Density Functional Theory (DFT) were employed to study the perovskite-type hydride LiSiH3, to gain detailed insights into its structural, electronic, dynamic, and mechanical properties. The results confirmed that the material is stable. LiSiH3 has a gravimetric hydrogen storage capacity of about 7.94 wt, showing good potential for solid-state hydrogen storage. These results provide a clear understanding of the material and demonstrate how structural tuning can enhance its performance for future hydrogen-based energy applications.

Effect of Mn3+ substitution by Fe3+ on the magnetocaloric effect of La0.9M0.1MnO3 (M=Na; Li)

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Abstract

The thermal, structural, magnetic, and magnetocaloric properties of 10% Fe-doped $La_{0.9}A_{0.1}MnO_3$ (A = Na, Li) perovskite manganites prepared by the Flash combustion method were studied in this work. These materials were characterized by thermogravimetric analysis, X-ray diffraction at room temperature, and magnetization measurements versus temperature and under different applied magnetic fields. The Fe-doped $La_{0.9}A_{0.1}MnO_3$ (A = Na, Li) crystallized in rhombohedral symmetry with $R\bar{3}c$ space group. Furthermore, the magnetization curves indicate that all samples undergo a magnetic transition at the Curie temperature T_C from the paramagnetic to the ferromagnetic phase. This study reinforces the concept that T_C and the magnetic entropy decrease upon replacing Mn with Fe, and no transformation from rhombohedral to cubic or orthorhombic symmetry was observed. The changes in the magnetocaloric properties are interpreted based on the fact that substitution of Mn^{3+} by Fe^{3+} reduces

the number of Mn sites, which weakens the double-exchange (DE) interactions between Mn^{3+} and Mn^{4+} ions.

Quantifying Non-Classical Correlations via Linear-Entropy Quantum Discord in Qubit–Qutrit Systems

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Abstract

We develop a robust analytical approach for quantifying non-classical correlations in general qubit–qutrit states using linear entropy. This entropy measure allows us to circumvent the optimization issues associated with classical correlations when quantum discord is defined via the von Neumann entropy. The linear entropy based quantum discord is then applied to characterize quantum correlations in a mixed spin qubit-qutrit system at thermal equilibrium at temperature. We further examine the behavior of the system in the presence of an external magnetic field. The resulting quantum discord is compared with measurement-induced disturbance (MID) and logarithmic negativity. Our analysis reveals that both QD and MID exhibit greater robustness to thermal and environmental effects than entanglement and that they can be effectively used to identify the critical points of quantum phase transitions in the system.

Multicolor Emission in LaPO4:Ce3+/Mn2+ via Zr4+ Co-Doping for Lighting Applications

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Abstract

In this work, Zr^{4+}-modified $LaPO_4$:Ce^{3+}/Mn^{2+} (LPOCM) phosphors were prepared through a simple co-precipitation method to achieve tunable multicolor emission. All samples crystallize in a monoclinic $LaPO_4$ structure and show rod-like shapes. The impact of Zr^{4+} co-doping on the optical behavior was investigated using photoluminescence (PL) and electron paramagnetic resonance (EPR) spectroscopy. Systematic variations in excitation/emission profiles, decay lifetimes, and energy transfer efficiency ($Ce^{3+} \rightarrow Mn^{2+}$) were observed with increasing Zr^{4+} content. Under Ce^{3+} UV excitation, the materials display a green-to-red Mn^{2+} emission coming from the $^4T_1(G) \rightarrow {}^6A_1(S)$ transition, while charge compensation induced by Zr^{4+} enhances Mn^{2+} emission intensity and gives adjusted colors. The Ce^{3+}-only phosphor

exhibits intense blue emission with high color purity (97%). By introducing 5% Zr^{4+}, a near-ideal cold white emission is achieved with CIE 1931 coordinates (0.309, 0.329), close to standard white (0.330, 0.330). Higher Zr^{4+} concentrations shift the emission toward warm white and orange-red tones. These results highlight Zr^{4+} co-doping as an efficient strategy for enhancing luminescence and achieving broad color tunability in LPOCM phosphors for lighting applications.

Valorization of Waste in Mortars: Impacts on Durability and Energy Efficiency

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Abstract

The valorization of waste materials in mortars offers a sustainable solution to reduce the environmental impact of the construction sector. Incorporating industrial, agricultural, or plastic waste limits the use of traditional raw materials while providing valuable functional properties. These recycled components help reduce thermal conductivity, thereby improving the energy efficiency of buildings. However, their addition alters the mortar's microstructure and may affect mechanical strength, durability, and long-term stability. Recent studies show that optimized mix designs and appropriate waste treatments can achieve a suitable balance between thermal and mechanical performance. This approach paves the way for more eco-friendly and innovative mortars that meet the requirements of sustainable construction.

Landau Level Structure and Quantized Hall Conductivity of multi-Weyl Semimetal

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Abstract

We analyze the Landau level structure of a multi-Weyl semimetal and its impact on the Hall conductivity. In the zero-anisotropy limit, the effective model reduces to an isotropic Hamiltonian, enabling a direct comparison between isotropic and anisotropic regimes. Using Kubo's formalism, we compute the Hall conductivity σ_{xy} for different topological charges and various values of the chemical potential. We show that the quantized Hall conductivity σ_{xy}, as a function of the reduced chemical potential μ_r, exhibits a plateau structure: the resulting staircase reflects the sequential filling of Landau levels, with a central step enlarged by the zero modes characteristic of multi-Weyl fermions.

Advanced Quantum Dot Materials for Biomedical and Energy Applications

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Abstract

Quantum dots (QDs) have emerged as highly versatile nanostructures whose tunable optical and electronic properties open new perspectives in both biomedical and energy-related technologies. Their size-dependent behavior enables precise control of light absorption, charge transport and emission processes, making them attractive for applications ranging from targeted bioimaging and medical diagnostics to solar energy harvesting and photocatalysis. This poster presents an overview of recent advances in the design, synthesis and functionalization of quantum dots, with emphasis on how their structure–property relationships can be engineered to meet specific requirements in health and energy systems. Particular attention is given to the integration of QDs into hybrid devices, the improvement of their stability and biocompatibility, and their role in enhancing sensor performance and energy conversion efficiency. These developments highlight the growing potential of quantum dots as key materials for next-generation biomedical tools and sustainable energy solutions.

Efficient in-vitro quality assurance for head-and-neck radiation therapy using optically stimulated luminescence dosimeters

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Abstract

Background and purpose: Head-and-neck (HN) radiotherapy treatment planning is highly complex process due to critical structures close to the target volume, which leads to significant uncertainties between calculated and delivered dose distributions. We establish an efficient end-to-end quality-assurance protocol to assess the overall treatment chain uncertainty and accuracy, and to ensure reliable workflow. Materials and Methods: 4 VMAT treatment plans of the HN cancers were selected based on their clinical incidence frequency, with a proscribed dose of 2Gy per fraction. An anthropomorphic phantom was used for measurement, mimicking patient anatomy in

real-world scenario starting from CT-imaging, through dose calculation on the treatment planning system (TPS), to plans administration under the LINAC. A batch of OSL detectors were first calibrated on the same treatment conditions to minimize detectors signal variation. The selected treatment plans were applied to the phantom as QA-Plans to keep the same plan parameters and then measure in real-world conditions. Each measurement was repeated numerous times to reduce statistical uncertainties, and the mean absorbed dose was recorded. Results: The mean dose discrepancy (±SD) between TPS and OSLD was 0.76 ± 2.22, 0.68 ± 4.51, 1.56 ± 2.85, and 2.04 ± 3.53 for brain metastases, parotid glans, nasopharyngeal and laryngeal cancers respectively. Plans standard deviations SDTPS–OSLD increased with the mean dose difference Max–min, reflecting the effect of dose heterogeneity at measurement points. Over all plans, a lower difference of about 0.72 was shown between the highest and the lowest in-field standard deviation SDin () indicating the homogeneity level of dose inside the tumor volumes. Out-of-field standard deviations SDout() indicated a higher dose discrepancy due to organ at risk to be spared. Conclusion: VMAT treatment planning for head-and-neck cancers is highly complex, with numerous uncertainties that can compromise delivery accuracy. Implementing an end-to-end test is therefore essential to verify the system's ability to meet therapeutic objectives while sparing organs at risk

Modeling and Simulation of Quantum Key Distribution Protocols

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Abstract

This poster presents preliminary work on the modeling and simulation of quantum key distribution (QKD) protocols. The objective is to understand how noise, losses, and decoherence affect the performance and security of protocols such as BB84 and Twin-Field QKD. Numerical tools are used to explore realistic channel conditions and evaluate the behavior of quantum states during transmission. These early simulations serve as a foundation for developing more advanced models and for guiding future improvements in quantum communication systems

Demonstrating an unconditional separation between quantum and classical information resources

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Abstract

A longstanding goal in quantum information science is to demonstrate quantum computations that cannot be feasibly reproduced on a classical computer. Such demonstrations mark major milestones: they showcase fine control over quantum systems and are prerequisites for useful quantum computation. To date, quantum advantage has been demonstrated, for example, through violations of Bell inequalities and sampling-based quantum supremacy experiments. However, both forms of

advantage come with important caveats: Bell tests are not computationally difficult tasks, and the classical hardness of sampling experiments relies on unproven complexity-theoretic assumptions. Here we demonstrate an unconditional quantum advantage in information resources required for a computational task, realized on Quantinuum's H1-1 trapped-ion quantum computer operating at a median two-qubit partial-entangler fidelity of 99.941(7). We construct a task for which the most space-efficient classical algorithm provably requires between 62 and 382 bits of memory, and solve it using only 12 qubits. Our result provides the most direct evidence yet that currently existing quantum processors can generate and manipulate entangled states of sufficient complexity to access the exponentiality of Hilbert space. This form of quantum advantage — which we call quantum information supremacy — represents a new benchmark in quantum computing, one that does not rely on unproven conjecture

Experimental and DFT Investigation of Ni-doped LaCoO3 Nanoparticles: Structure, Morphology and Electronic Properties

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Abstract

This research focuses on enhancing the structure, electronic and magnetic properties of the perovskite material lanthanum cobalt oxide (LaCoO3) for application in devices like sensors and data storage. The project involves synthesizing LaCoO3 where cobalt is partially doped with nickel Ni, creating LaCo1x NixO3. The synthesized material is then characterized using XRD, SEM, TEM, and FTIR to analyze its structure, composition behavior. Finally, Density Functional Theory (DFT) simulations are used to model the material's electronic structure at the atomic level, providing a theoretical understanding of how nickel doping alters its magnetic and electronic properties.

Performance analysis of CaZrS3-based chalcogenide perovskite solar cells with theoretical efficiency approaching 35

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Abstract

Photovoltaic limited efficiency and the high cost of silicon solar cells are key issues for the solar cell to become an alternative to the use of readily available fossil fuels. Therefore, the development of new cost-effective and non-toxic photovoltaic materials and energy-efficient processes is essential. Chalcogenide perovskites have great potential to fulfill these requirements. Among them is CaZrS3. In this study, a device simulation

of CaZrS3 material is reported for the first time, which makes this new study interesting, using the one-dimensional solar cell capacitance simulator SCAPS-1D. Therefore, we tried to propose low-cost Electron Transport Materials ETMs (TiO2, ZnO, and SnO2). The influence of thickness, doping concentration (NA), and the working temperature on the device performance was studied. To enhance the cell Power Conversion Efficiency (PCE), optimization of the device design's key parameters is performed.

Thermo-electrochemical modeling of fuel cells for hydrogen-to power conversion

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Abstract

Proton Exchange Membrane Fuel Cells (PEMFCs) convert hydrogen into electricity with zero emissions and high energy density. However, nearly half of the input energy is released as heat, causing membrane dehydration, efficiency losses, and material degradation, making thermal management essential. This work presents a dynamic thermo-electrochemical model of a water-cooled PEMFC, with 3D geometry designed in CAD and governing equations implemented in Python, validated experimentally to study temperature effects and optimize cooling. Results show that the approach regulates cell temperature, enhances power output over time, contributing to long-term stability and durability.

Modeling and Optimization of Renewable Energy Systems for Power Generation and Hydrogen Production

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Abstract

This study analyzes green hydrogen production in Morocco using hybrid photovoltaic–wind systems, with and without battery energy storage. An hourly dynamic model is developed using Python language to evaluate the effects of renewable resource availability, electrolyzer sizing, and storage strategies on system performance and hydrogen costs. Two scenarios are analyzed, one with battery storage system to store the excess produced energy, and the other without energy storage. Among five studied sites in Morocco, Dakhla shows the best potential, achieving the lowest Levelized Cost of green Hydrogen: 3.16 $/kgHwithoutbatteriesstorageand$3.87/kg H with batteries storage.

Artificial Intelligence-Based Approach for Modeling Thermochemical Storage Systems

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Abstract

This project applies artificial intelligence—mainly machine learning and artificial neural networks—to model a thermochemical heat storage system based on zeolite–water adsorption. Experimental data from the CETHIL laboratory are combined with advanced AI models, including LSTM and hybrid FNN-LSTM networks, to predict the thermal behavior of the reactor with high accuracy. The approach provides reliable temperature forecasting and demonstrates the ability of AI to support effective control of thermochemical systems. The work also opens perspectives for physics-informed neural networks, real-time monitoring, and improved energy storage solutions for sustainable building technologies.

Ab Initio Study of the Electronic, Thermodynamic, Thermoelectric, and Optical Properties of HfSeS in the (100), (110), and (111) Crystallographic Directions

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Abstract

In this article, we present a comprehensive theoretical investigation of the structural, electronic, thermodynamic, thermoelectric, and optical properties of the HfSeS compound along the (100), (110), and (111) crystallographic directions. These properties are examined using density functional theory (DFT) within the Generalized Gradient Approximation (GGA), and spin–orbit coupling (SOC) is also included due to the presence of heavy atoms in the compound. The electronic structure calculations show that HfSeS exhibits an indirect M– band gap for all crystallographic orientations, with a strong consistency observed between the GGA and SOC results. To gain deeper insight into the optical response of the material under external constraints, the optical properties are further analyzed under applied hydrostatic pressure. The thermodynamic behavior of HfSeS is investigated through the quasi-harmonic Debye model implemented in the Gibbs2 code, allowing the evaluation of key quantities such as heat capacities, thermal expansion coefficients, Debye temperature, and entropy over a broad range of pressures and temperatures. These results provide a detailed understanding of the material's performance under various thermodynamic conditions. Finally, the thermoelectric properties of HfSeS, including the Seebeck coefficient and electronic thermal conductivity, are computed to assess its potential for energy conversion

applications. Collectively, these analyses offer valuable insights into the fundamental physicochemical properties of HfSeS and highlight its potential functionalities across different technological domains.

Développement des Technologies de Conversion Energétique au Maroc

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Abstract

Le système « Power-to-Heat-to-X » avec stockage est un nouveau système qui permet de convertir l'énergie électrique, provenant principalement de sources renouvelables, en chaleur ou en énergie thermique. Cette énergie thermique peut être utilisée directement ou stockée dans un système de stockage de chaleur, puis convertie en différentes formes d'énergie, ce qui améliore la flexibilité et la durabilité du système énergétique. Cette étude fournit un aperçu des technologies PtHtX, notamment les processus Power-to-Heat, les solutions de stockage d'énergie thermique et les méthodes de conversion Heat-to-X qui transforment la chaleur en différents types d'énergie. L'article souligne le potentiel du Power-to-Heat-to-X au Maroc pour faire progresser la transition nationale vers des systèmes énergétiques durables et à faible émission de carbone

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