

# Abstracta

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**Artigos publicados**  
P116-2024 à P159-2024

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**Defesas de Teses do IFGW**  
T011-2024 à T012-2024

**Defesas do PECIM**  
P006-2024 à P007-2024

## Artigos publicados

### [P116-2024] “A comprehensive review of atomically thin silicates and their applications”

Mahapatra, P. L.; Costin, G.; Galvao, D. S.\*; Lahiri, B.; Glavin, N.; Roy, A. K.; Ajayan, P. M.; Tiwary, C. S.

Silicate is one of the most abundant minerals on Earth's crust and a sustainable source of two-dimensional (2D) complex oxides. In this review, we discuss the research progress of layered and non-layered 2D silicates, their comparison with conventional 2D materials, and a brief discussion on 2D silicate applications. The review begins with thoroughly examining synthesis strategies, emphasizing the various methods used to create layered and non-layered 2D silicates. The discussions then address the distinctive features of these materials, emphasizing their physicochemical characteristics. Furthermore, the review outlines recent breakthroughs in utilizing 2D silicates in electrical and memory devices, energy harvesting, energy storage, sensors, optoelectronics, water treatment, wound healing, cancer theranostics, bacterial ablation, fire retardancy, etc. By summarizing the most recent research findings in the field of 2D silicates and providing an overview of silicate evolution, this review intends to present a comprehensive resource for researchers interested in the diverse and fascinating area of 2D silicates.

2D MATERIALS 11[3], 032003, 2024. DOI: 10.1088/2053-1583/ad569b

### [P117-2024] “A source of entangled photons based on a cavity-enhanced and strain-tuned GaAs quantum dot”

Rota, M. B.; Krieger, T. M.; Buchinger, Q.; Beccaceci, M.; Neuwirth, J.; Huet, H.; Horová, N.; Lovicu, G.; Ronco, G.; Silva, S. F. C. da\*; Pettinari, G.; Moczala-Dusanowska, M.; Kohlberger, C.; Manna, S.; Stroj, S.; Freund, J.; Yuan, X. Y.; Schneider, C.; Jezek, M.; Höfling, S.; Basset, F. B.; Huber-Loyola, T.; Rastelli, A.; Trotta, R.

A quantum-light source that delivers photons with a high brightness and a high degree of entanglement is fundamental for the development of efficient entanglement-based quantum-key distribution systems. Among all possible candidates, epitaxial quantum dots are currently emerging as one of the brightest sources of highly entangled photons. However, the optimization of both brightness and entanglement currently requires different technologies that are difficult to combine in a scalable manner. In this work, we overcome this challenge by developing a novel device consisting of a quantum dot embedded in a circular Bragg resonator, in turn, integrated onto a micromachined piezoelectric actuator. The resonator engineers the light-matter interaction to empower extraction efficiencies up to 0.69(4). Simultaneously, the actuator manipulates strain fields that tune the quantum dot for the generation of entangled photons with corrected fidelities to a maximally entangled state up to 0.96(1). This hybrid technology has the potential to overcome the limitations of the key rates that plague QD-based entangled sources for entanglement-based quantum key distribution and entanglement-based quantum networks.

ELIGHT 4[1], 13, 2024. DOI: 10.1186/s43593-024-00072-8

### [P118-2024] “Adherence of p-Terphenyl (PTP) film on the dichroic filter used for the X-ARAPUCA device”

Mendonca, A. P. A.\*; Machado, A. A.\*; Marques, F. C.\*; Bazetto, M. C. Q.\*; Merlo, R. B.\*; Pierobao, C.\*; Figueroa, C. A.; Perotti, B. L.; Segreto, E.\*

The adherence of the p-Terphenyl film to the substrate in the X-ARAPUCA dichroic filter is directly correlated with the long-term efficiency and durability of this device. This study presents the results of different cleaning methods established to analyze their contributions to the film's adherence to the substrate. The samples underwent analysis of their crystalline and morphological structure using XRD and AFM techniques. Three distinct techniques were employed in the adherence tests: ultrasonic bath, scratch test, and cryogenic immersion method with turbulence, as these devices will be submerged in liquid argon in the DUNE experiment. Results suggest that the deposited PTP layer exhibits a monoclinic crystalline structure, with topography revealing percolated planar grains and roughness ranging from 13 nm to 18 nm. The various adherence techniques employed yielded consistent results, highlighting the standard cleaning process involving Soap + H<sub>2</sub>O + N<sub>2</sub> + Kiln as the preferred method.

JOURNAL OF INSTRUMENTATION 19[5], C05048, 2024. DOI: 10.1088/1748-0221/19/05/C05048

### [P119-2024] “Analysis of Macronutrients in Soil Using Impedimetric Multisensor Arrays”

Braunger, M. L.\*; Popolin Neto, M.; Kirsanov, D.; Fier, I.; Amaral, L. R.; Shimizu, F. M.\*; Correa, D. S.; Paulovich, F. V.; Legin, A.; Oliveira Jr., O. N.; Riul Jr., A.\*

The need to increase food production to address the world population growth can only be fulfilled with precision agriculture strategies to increase crop yield with minimal expansion of the cultivated area. One example is site-specific fertilization based on accurate monitoring of soil nutrient levels, which can be made more cost-effective using sensors. This study developed an impedimetric multisensor array using ion-selective membranes to analyze soil samples enriched with macronutrients (N, P, and K), which is compared with another array based on layer-by-layer films. The results obtained from both devices are analyzed with multidimensional projection techniques and machine learning methods, where a decision tree model algorithm chooses the calibrations (best frequencies and sensors). The multicalibration space method indicates that both devices effectively distinguished all soil samples tested, with the ion-selective membrane setup presenting a higher sensitivity to K content. These findings pave the way for more environmentally friendly and efficient agricultural practices, facilitating the mapping of cropping areas for precise fertilizer application and optimized crop yield.

ACS OMEGA, Early Access Date: JUL 2024. DOI: 10.1021/acsomega.4c04452

### [P120-2024] “Carbon quantum dots with ultra-high quantum yield for versatile turn-on sensor of gluten and cyanide ions”

Oliveira, J. J. P.; Carneiro, S. V.; Carvalho, E. F.; Rodrigues, V. S. F.; Lima, F. E. H.; Matos, W. O.; Fachine, L. M. U. D.; Antunes, R. A.; Neto, M. L. A.\*; Campos, A. T. P.; Moura, T. A.; Cesar, C. L.; Santos-Oliveira, R.; Carvalho, H. F.\*; Paschoal, A. R.; Freire, R. M.; Carvalho, C. J. R.; Fachine, P. B. A.

In this work, we reported the synthesis of carbon quantum dots (CQDs) with high fluorescent quantum yield (90.7 %). These nanoparticles were applied in a turn-off/turn-on sensor able to detect cyanide ions. In this sensing strategy, Fe<sup>3+</sup> ions were added to the aqueous suspension of CQDs to quench the fluorescence of the system, which was recovered from the presence of cyanide ions. Furthermore, a sensor array was developed using the LDA chemometric tool, to classify different species present in cookie formulations, including gluten.

The turnoff/turn-on sensor proved to be sensitive and effective for detecting cyanide ions, with a detection limit of 3.77 ppm. This high sensibility and selectivity allowed quantifying the analyte in a real sample of tap water.

**DYES AND PIGMENTS 229, 112312, 2024. DOI: 10.1016/j.dye-pig.2024.112312**

**[P121-2024] “Celestial sector in CFT: Conformally soft symmetries”**

Gioia, L. P. de\*; Raclariu, A. M.

We show that time intervals of width triangle tau in 3-dimensional conformal field theories (CFT3) on the Lorentzian cylinder admit an infinite dimensional symmetry enhancement in the limit triangle tau  $\rightarrow$  0. The associated vector fields are approximate solutions to the conformal Killing equations in the strip labelled by a function and a conformal Killing vector on the sphere. An Inonu-Wigner contraction yields a set of symmetry generators obeying the extended BMS4 algebra. We analyze the shadow stress tensor Ward identities in CFTd on the Lorentzian cylinder with all operator insertions in infinitesimal time intervals separated by pi. We demonstrate that both the leading and subleading conformally soft graviton theorems in (d - 1)-dimensional celestial CFT (CCFTd-1) can be recovered from the transverse traceless components of these Ward identities in the limit triangle tau  $\rightarrow$  0. A similar construction allows for the leading conformally soft gluon theorem in CCFTd-1 to be recovered from shadow current Ward identities in CFTd.

**SCIPOST PHYSICS 17[1], 002, 2024. DOI: 10.21468/SciPostPhys.17.1.002**

**[P122-2024] “Charge amplification in low pressure CF4:SF6:He mixtures with a multi-mesh ThGEM for directional dark matter searches”**

Amaro, F. D.; Baracchini, E.; Monteiro, C. M. B.\*; et al.

The CYGNO collaboration is developing next generation directional Dark Matter (DM) detection experiments, using gaseous Time Projection Chambers (TPCs), as a robust method for identifying Weakly Interacting Massive Particles (WIMPs) below the Neutrino Fog. SF 6 is potentially ideal for this since it provides a high fluorine content, enhancing sensitivity to spin -dependent interactions and, as a Negative Ion Drift (NID) gas, reduces charge diffusion leading to improved positional resolution. CF 4 , although not a NID gas, has also been identified as a favourable gas target as it provides a scintillation signal which can be used for a complimentary light/charge readout approach. These gases can operate at low pressures to elongate Nuclear Recoil (NR) tracks and facilitate directional measurements. In principle, He could be added to low pressure SF 6 /CF 4 without significant detriment to the length of 16 S, 12 C, and 19 F recoils. This would improve the target mass, sensitivity to lower WIMP masses, and offer the possibility of atmospheric operation; potentially reducing the cost of a containment vessel. In this article, we present gas gain and energy resolution measurements, taken with a Multi-Mesh Thick Gaseous Electron Multiplier (MMThGEM), in low pressure SF 6 and CF 4 :SF 6 mixtures following the addition of He. We find that the CF 4 :SF 6 :He mixtures tested were able to produce gas gains on the order of 10 4 up to a total pressure of 100 Torr. These results demonstrate an order of magnitude improvement [1] in charge amplification in NID gas mixtures with a He component.

**JOURNAL OF INSTRUMENTATION 19[6], P06021, 2024. DOI: 10.1088/1748-0221/19/06/P06021**

**[P123-2024] “Constraints on metastable superheavy dark matter coupled to sterile neutrinos with the Pierre Auger Observatory”**

Halim, A. A.; Abreu, P.; Arbeletche, L. B.\*; Chinellato, J. A.\*; Dobrigkeit, C.\*; Fauth, A. C.\*; Payeras, A. M.\*; Akim, J. V. R.\*; et al.  
Pierre Auger Collaboration

Dark matter particles could be superheavy, provided their lifetime is much longer than the age of the Universe. Using the sensitivity of the Pierre Auger Observatory to ultrahigh energy neutrinos and photons, we constrain a specific extension of the Standard Model of particle physics that meets the lifetime requirement for a superheavy particle by coupling it to a sector of ultralight sterile neutrinos. Our results show that, for a typical dark coupling constant of 0.1, the mixing angle  $\theta$  between active and sterile neutrinos must satisfy, roughly,  $\theta < 1.5 \times 10^{-6} (M_X/10^9 \text{ GeV})^{-2}$  for a mass  $M_X$  of the dark-matter particle between  $10^8 \text{ GeV}$  and  $10^{11} \text{ GeV}$ .

**PHYSICAL REVIEW D 109[8], L081101, 2024**

**[P124-2024] “Control of Anisotropy and Magnetic Hyperthermia Effect by Addition of Cobalt on Magnetite Nanoparticles”**

Almeida, A. A. de\*; Fabris, F.\*; Silva, G. S. da\*; Pirota, K. R.\*; Knobel, M.\*; Muraca, D.\*

Magnetic hyperthermia (MH) has emerged as a promising technology with diverse applications in medical and technological fields, leveraging the remote induction of temperature elevation through an alternating magnetic field. While Fe<sub>3</sub>O<sub>4</sub> nanoparticles with an average size around 12-25 nm are commonly employed in MH systems, this study introduces a strategy to produce smaller particles (less than or equal to 10 nm) with enhanced heating efficiency, as measured by specific power absorption (SPA). We conducted an exhaustive and detailed investigation into the morphological and magnetic properties of CoFe<sub>3-x</sub>O<sub>4</sub> nanoparticles, aiming to optimize their MH response. By varying the Co content, we successfully tuned the effective magnetic anisotropy while maintaining saturation magnetization nearly constant. The MH analysis indicates that these nanoparticles predominantly heat through the Neel mechanism, demonstrating robust reproducibility across different concentrations, viscosity mediums, and ac field conditions. Notably, we identified an optimal anisotropy or Co concentration that maximizes SPA, crucial for developing magnetic systems requiring particles with specific sizes. This work contributes to advancing the understanding and application of MH, particularly in tailoring nanoparticle properties for targeted and efficient heat generation in various contexts.

**ACS APPLIED MATERIALS & INTERFACES, Early Access Date: JUL 2024. DOI: 10.1021/acsami.4c03343**

**[P125-2024] “Controlled Insertion of Silver Nanoparticles in LbL Nanostructures: Fine-Tuning the Sensing Units of an Impedimetric E-Tongue”**

Gonçalves, M. H.\*; Braunger, M. L.\*; Barros, A. de; Hensel, R. C.; Dalafini, J. G.\*; Mazali, I. O.; Correa, L. M.\*; Ugarte, D.\*; Riul Jr., A.\*; Rodrigues, V.\*

Silver nanoparticles (AgNPs) possess unique characteristics ideal for enhancing device sensitivity, primarily due to their high surface-to-volume ratio facilitating heightened interaction with analytes. Integrating AgNPs into polymers or carbon-based materials results in nanocomposites with synergistic properties, enabling the detection of minute changes in the environment across various applications.

In this study, we investigate the adsorption kinetics of AgNPs within multilayered layer-by-layer (LbL) structures, specifically examining the impact of AgNPs concentration in the LbL film formation that is further explored as sensing units in an impedimetric microfluidic e-tongue. Although absorption kinetic studies are infrequent, they are crucial to optimize the AgNPs adsorption and distribution within LbL structures, significantly influencing upcoming applications. Through systematic variation of AgNPs concentration within identical LbL architectures, we applied the films as sensing units in a microfluidic e-tongue capable of distinguishing food enhancers sharing the umami taste profile. Across all tested scenarios, our approach consistently achieves robust sample separation, evidenced by silhouette coefficient, principal component analyses, and long-term stability. This work contributes to exploring controlled nanomaterial-based developments, emphasizing the importance of precise parameter control for enhanced sensor performance across diverse analytical applications.

**CHEMOSENSORS 12[6], 87, 2024. DOI: 10.3390/chemosensors12060087**

**[P126-2024] “Detection of Psychoactive N,N-Dimethyltryptamine Alkaloid Based on Surface-Enhanced Raman Scattering Using Gold Nanostars in Flexible Inkjet-Printing Paper Substrates”**

Huertas-Montoya, E.; Barros, A. de; Oliveira, L. M. F.; Aponte, P. A. C.; Oliveira, A. L. R.; Shimizu, F. M.\*; Sussulini, A.; Sigoli, F. A.; Mazali, I. O.

N,N-Dimethyltryptamine (DMT) is a serotonergic psychedelic that, when combined with monoamine oxidase enzyme inhibitors in the hallucinogenic beverage commonly known as ayahuasca, surpasses most common orally administered psychoactive drugs. There is a growing interest in the therapeutic potential of DMT due to recent clinical data showing the improvement of cognitive deficits associated with depression and Alzheimer’s disease. The development of analytical methodology for the monitoring of concentrations of DMT molecules to control the appropriate dosage for their use is essential for the treatment of patients. For this, we propose a novel flexible inkjet-printed paper substrate based on Au nanostars as proof of concept for DMT detection by surface-enhanced Raman scattering (SERS). The substrate was applied to detect DMT in water as a first approach to more complex matrices like ayahuasca beverages or blood samples. The optimization and performance of SERS substrates with different print cycles indicate that one print is enough to achieve the great performance of the flexible paper substrates. The SERS analyses for DMT in different concentrations, 10<sup>-3</sup> to 10<sup>-10</sup> mol L<sup>-1</sup>, reveal a high sensitivity of the sensors with a silhouette coefficient of 0.84 obtained by principal component analysis (PCA) statistical projections.

**JOURNAL OF THE BRAZILIAN CHEMICAL SOCIETY 35[12], e20240105, 2024. DOI: 10.21577/0103-5053.20240105**

**[P127-2024] “Differences between Alzheimer’s disease and mild cognitive impairment using brain networks from magnetic resonance texture analysis”**

Silveira, R. V. da\*; Magalhaes, T. N. C.; Balthazar, M. L. F.; Castellano, G.\*

Several studies have aimed at identifying biomarkers in the initial phases of Alzheimer’s disease (AD). Conversely, texture features, such as those from gray-level co-occurrence matrices (GLCMs), have highlighted important information from several types of medical images. More recently, texture-based brain networks have been shown to provide useful information in characterizing healthy individuals.

However, no studies have yet explored the use of this type of network in the context of AD. This work aimed to employ texture brain networks to investigate the distinction between groups of patients with amnesic mild cognitive impairment (aMCI) and mild dementia due to AD, and a group of healthy subjects. Magnetic resonance (MR) images from the three groups acquired at two instances were used. Images were segmented and GLCM texture parameters were calculated for each region. Structural brain networks were generated using regions as nodes and the similarity among texture parameters as links, and graph theory was used to compute five network measures. An ANCOVA was performed for each network measure to assess statistical differences between groups. The thalamus showed significant differences between aMCI and AD patients for four network measures for the right hemisphere and one network measure for the left hemisphere. There were also significant differences between controls and AD patients for the left hippocampus, right superior parietal lobule, and right thalamus-one network measure each. These findings represent changes in the texture of these regions which can be associated with the cortical volume and thickness atrophies reported in the literature for AD. The texture networks showed potential to differentiate between aMCI and AD patients, as well as between controls and AD patients, offering a new tool to help understand these conditions and eventually aid early intervention and personalized treatment, thereby improving patient outcomes and advancing AD research.

**EXPERIMENTAL BRAIN RESEARCH 242[8], 1947-1955, 2024. DOI: 10.1007/s00221-024-06871-2**

**[P128-2024] “Enhanced Diagnostic Precision: Assessing Tumor Differentiation in Head and Neck Squamous Cell Carcinoma Using Multi-Slice Spiral CT Texture Analysis”**

Oliveira, L. A. P. de; Lopes, D. L. L.; Gomes, J. P. P.; Silveira, R. V. da\*; Nozaki, D. V. de A.; Santos, L. F.; Castellano, G.\*; Lopes, S. L. P. de C.; Costa, A. L. F.

This study explores the efficacy of texture analysis by using preoperative multi-slice spiral computed tomography (MSCT) to non-invasively determine the grade of cellular differentiation in head and neck squamous cell carcinoma (HNSCC). In a retrospective study, MSCT scans of patients with HNSCC were analyzed and classified based on its histological grade as moderately differentiated, well-differentiated, or poorly differentiated. The location of the tumor was categorized as either in the bone or in soft tissues. Segmentation of the lesion areas was conducted, followed by texture analysis. Eleven GLCM parameters across five different distances were calculated. Median values and correlations of texture parameters were examined in relation to tumor differentiation grade by using Spearman’s correlation coefficient and Kruskal-Wallis and Dunn tests. Forty-six patients were included, predominantly female (87%), with a mean age of 66.7 years. Texture analysis revealed significant parameter correlations with histopathological grades of tumor differentiation. The study identified no significant age correlation with tumor differentiation, which underscores the potential of texture analysis as an age-independent biomarker. The strong correlations between texture parameters and histopathological grades support the integration of this technique into the clinical decision-making process.

**JOURNAL OF CLINICAL MEDICINE 13[14], 4038, 2024. DOI: 10.3390/jcm13144038**

**[P129-2024] “Enhancing UV Radiation Resilience of DLC-Coated Stainless Steel with TiO<sub>2</sub>: A Dual-Layer Approach”**

Macário, P. F.; Silveira, C. H. da; Vieira, A. A. M.; Marcondes, A. R.; Marques, F. das C.\*; Fehine, G. J. M.; Vieira, L.

This study presents an innovative dual-layer coating approach integrating titanium dioxide (TiO<sub>2</sub>) onto diamond-like carbon (DLC)-coated 316L stainless steel. The combination of PECVD-deposited DLC and ALD-deposited TiO<sub>2</sub> aims to preserve the inherent tribological properties of DLC while mitigating UV-induced degradation. By leveraging the ability of TiO<sub>2</sub> to absorb, reflect, and scatter UV light, this dual-layer strategy significantly enhances the durability of DLC coatings in radiation-prone environments. The effects of accelerated aging through UV exposure on DLC and DLC/TiO<sub>2</sub> films were evaluated using an Accelerated Weathering Tester. Comprehensive analyses were conducted to assess the structural and mechanical properties before and after UV exposure, including Raman spectroscopy, profilometry, SEM, EDS, nanoindentation, and tribometry. The results demonstrate that the TiO<sub>2</sub> layer effectively mitigates UV-induced damage, preserving the DLC film's integrity and tribological performance even after 408 h of UV aging. Specifically, the DLC/TiO<sub>2</sub> coatings maintained lower roughness, higher hardness, and better adhesion than DLC-only coatings under identical conditions. This research significantly advances protective coating technology by enhancing the durability and performance of DLC films, particularly in aerospace and other demanding industries where exposure to UV radiation is a critical concern.

COATINGS 14[6], 777, 2024. DOI: 10.3390/coatings14060777

#### [P130-2024] “Ferroelectricity-Induced Surface Ferromagnetism in Core-Shell Magnetoelectric Nanoparticles”

Canhassi, C. A. I.\*; Chernozem, R. V.; Chernozem, P. V.; Romanyuk, K. N.; Zelenovskiy, P.; Urakova, A. O.; Gerasimov, E. Y.; Koptsev, D. A.; Surmeneva, M. A.; Surmenev, R. A.; Kholkin, A. L.; Kopelevich, Y.\*

Magnetoelectric nanoparticles (NPs) present an important class of nanomaterials with a wide interest in piezocatalytic and biomedical applications. Herein, the results of magnetoelectric and magnetization measurements performed on core-shell NPs having magnetic core (MnFe<sub>2</sub>O<sub>4</sub>, MFO) and ferroelectric shell (Ba<sub>0.85</sub>Ca<sub>0.15</sub>Ti<sub>0.5</sub>Zr<sub>0.5</sub>O<sub>3</sub>, BCZT) synthesized by the microwave hydrothermal method are reported. Magnetic results are compared with the measurements on reference MFO NPs prepared under identical conditions. Detailed SQUID magnetometer measurements of the magnetization hysteresis loops  $M(H)$  down to 2 K reveal the existence of a clear exchange bias effect in pure MFO NPs attributed to the coexistence of ferromagnetic and antiferromagnetic short-range interactions. When the magnetic core is covered by the thin ferroelectric BCZT shell, it is observed that 1) the shell suppresses the apparent bias effect and 2) induces an “extra” ferromagnetic magnetization at  $T < 20$  K. The results indicate that this “extra” ferromagnetism has a 2D character and it is most likely related to the interface interactions between the MFO core and BCZT shell. Ferroelectric properties and strong magnetoelectric effect in core-shell NPs are revealed via piezoresponse force microscopy under magnetic field. The mechanisms of the observed effects are discussed.

PHYSICA STATUS SOLIDI-RAPID RESEARCH LETTERS, Early Access Date: JUL 2024. DOI: 10.1002/psr.202400122

#### [P131-2024] “First Measurement of the $|t|$ Dependence of Incoherent $J/\psi$ Photonuclear Production”

Acharya, S.; Adamová, D.; Chinellato, D. D.\*; Guardiano, G. G.\*; Jahnke, C.\*; Liveraro, G. S. S.\*; Takahashi, J.\*; et al. ALICE Collaboration

The first measurement of the cross section for incoherent photonuclear production of  $J/\psi$  vector mesons as a function of the Mandelstam  $t$  variable is presented.

The measurement was carried out with the ALICE detector at midrapidity, vertical bar  $t$  vertical bar  $< 0.8$ , using ultraperipheral collisions of Pb nuclei at a center-of-mass energy per nucleon pair of  $\sqrt{s_{NN}} = 5.02$  TeV. This rapidity interval corresponds to a Bjorken- $x$  range  $0.3-1.4 \times 10^{-3}$ . Cross sections are given in five  $t$  intervals in the range  $0.04 < \text{vertical bar } t \text{ vertical bar} < 1$  GeV<sup>2</sup> and compared to the predictions by different models. Models that ignore quantum fluctuations of the gluon density in the colliding hadron predict a  $t$  dependence of the cross section much steeper than in data. The inclusion of such fluctuations in the same models provides a better description of the data.

PHYSICAL REVIEW LETTERS 132[16], 2024. DOI: 10.1103/PhysRevLett.132.162302

#### [P132-2024] “Four-gluon vertex in collinear kinematics”

Aguilar, A. C.\*; Ferreira, M. N.; Papavassiliou, J.; Santos, L. R.\*

To date, the four-gluon vertex is the least explored component of the QCD Lagrangian, mainly due to the vast proliferation of Lorentz and color structures required for its description. In this work we present a nonperturbative study of this vertex, based on the one-loop dressed Schwinger-Dyson equation obtained from the 4PI effective action. A vast simplification is brought about by resorting to “collinear” kinematics, where all momenta are parallel to each other, and by appealing to the charge conjugation symmetry in order to eliminate certain color structures. Out of the fifteen form factors that comprise the transversely-projected version of this vertex, two are singled out and studied in detail; the one associated with the classical tensorial structure is moderately suppressed in the infrared regime, while the other diverges logarithmically at the origin. Quite interestingly, both form factors display the property known as “planar degeneracy” at a rather high level of accuracy. With these results we construct an effective charge that quantifies the strength of the four-gluon interaction, and compare it with other vertex-derived charges from the gauge sector of QCD.

EUROPEAN PHYSICAL JOURNAL C 84[7], 676, 2024. DOI: 10.1140/epjc/s10052-024-12970-9

#### [P133-2024] “Graph network and symmetry analysis after combined XR and tDCS in stroke rehabilitation”

Carlos, B. M.\*; Menezes, L. T.\*; Rosa, B.\*; Furumoto, B. F.\*; Feitosa, S. S.\*; Fernandes, C. A.; Ferreira-Melo, S. E.; Pereira, J. D.\*; Almeida, S.\*; Brandao, A. F.; Ruas, C. V.\*; Castellano, G.\*

The integration of innovative neurotechnologies in rehabilitation programs seems promising for enhancing motor recovery in people with stroke. This study presents a comprehensive exploration of brain connectivity with symmetry and graph network analyses during motor rehabilitation using extended reality (XR) training and transcranial direct current stimulation (tDCS). The evolution of selected electroencephalography (EEG) features was assessed along with changes in clinical scores before and after the rehabilitation program in order to identify directions for future research. Clinical motor performance scales and resting-state EEG assessments showed trends indicating the improvement of connectivity and integration capacity over rehabilitation time, particularly within the theta, beta, and gamma frequency bands. Symmetry indices, particularly at higher frequencies, were significantly correlated with clinical improvements, demonstrating a stronger relationship between brain symmetry and lower extremity function as well as an increasing symmetry trend at the end of the rehabilitation program. Based upon the preliminary findings of this study, rehabilitation sessions that combine XR and tDCS can induce changes in neuroplasticity and improve motor recovery, which may in turn increase the life quality of people with stroke.

[P134-2024] “Graph network and symmetry analysis after combined XR and tDCS in stroke”

Carlos, B. M.\*; Menezes, L. T.\*; Rosa, B.\*; Furumoto, B. F.\*; Feitosa, S. S.\*; Fernandes, C. A.; Ferreira-Melo, S. E.; Pereira, J. D.\*; Almeida, S.\*; Brandao, A. F.; Ruas, C. V.\*; Castellano, G.\*

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[P135-2024] “Ground observations of a space laser for the assessment of its in-orbit performance”

Lux, O.; Krisch, I.; Arbeletche, L. B.; Chinellato, J. A.\*; Franco, D. de O.\*; Dobrigkeit, C.\*; Fauth, A. C.\*; Payeras, A. M.\*; Akim, J. V. R.\*; et al.  
Pierre Auger Collaboration

The wind mission Aeolus of the European Space Agency was a groundbreaking achievement for Earth observation. Between 2018 and 2023, the space -borne lidar instrument ALADIN onboard the Aeolus satellite measured atmospheric wind profiles with global coverage, which contributed to improving the accuracy of numerical weather prediction. The precision of the wind observations, however, declined over the course of the mission due to a progressive loss of the atmospheric backscatter signal. The analysis of the root cause was supported by the Pierre Auger Observatory in Argentina whose fluorescence detector registered the ultraviolet laser pulses emitted from the instrument in space, thereby offering an estimation of the laser energy at the exit of the instrument for several days in 2019, 2020, and 2021. The reconstruction of the laser beam not only allowed for an independent assessment of the Aeolus performance, but also helped to improve the accuracy in the determination of the laser beam’s ground track on single pulse level. The results presented in this paper set a precedent for the monitoring of space lasers by ground -based telescopes and open new possibilities for the calibration of cosmic -ray observatories. Published by Optica Publishing Group under the terms of the Creative Commons Attribution 4.0 License. Further distribution of this work must maintain attribution to the author(s) and the published article’s title, journal citation, and DOI.

[P136-2024] “Higher-order moments of the elliptic flow distribution in PbPb collisions at  $\sqrt{s_{NN}}=5.02$  TeV”

Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; et al.  
CMS Collaboration

The hydrodynamic flow-like behavior of charged hadrons in high-energy lead-lead collisions is studied through multiparticle correlations. The elliptic anisotropy values based on different orders of multiparticle cumulants,  $v(2)\{2k\}$ , are measured up to the tenth order ( $k = 5$ ) as functions of the collision centrality at a nucleon-nucleon center-of-mass energy of  $\sqrt{s_{NN}} = 5.02$  TeV. The data were recorded by the CMS experiment at the LHC and correspond to an integrated luminosity of  $0.607 \text{ nb}^{-1}$ . A hierarchy is observed between the coefficients, with  $v(2)\{2\} > v(2)\{4\}$  greater than or similar to  $v(2)\{6\}$  greater than or similar to  $v(2)\{8\}$  greater than or similar to  $v(2)\{10\}$ . Based on these results, centrality-dependent moments for the fluctuation-driven event-by-event  $v(2)$  distribution are determined, including the skewness, kurtosis and, for the first time, superskewness. Assuming a hydrodynamic expansion of the produced medium, these moments directly probe the initial-state geometry in high-energy nucleus-nucleus collisions.

[P137-2024] “Illuminating Pathways to Dynamic Nanotribology: Light-Mediated Active Control of Interfacial Friction with Nanosuspensions”

Leidens, L. M.\*; Michels, A. F.; Machado, G.; Alvarez, F.\*; Smirnov, A. I.; Krim, J.; Figueroa, C. A.

Active control of nanotribological properties is a challenge. Materials responsive to external stimuli may catalyze this paradigm shift. Recently, the nanofriction of a thin film is modulated by light, ushering in phototribology. This frontier is expanded here, by investigating photoactive nanoparticles in lubricants to confer similar functionality to passive surfaces. Quartz-crystal microbalance (QCM) is employed to assess the phototribological behavior of aqueous suspensions of titanium dioxide nanoparticles. A comparison of dark and illuminated conditions provides the first demonstration of tuning the interfacial friction in solid-nanosuspension interfaces by light. Cyclic tests reveal reversible transitions between higher (dark) and lower friction (illuminated) regimes. These transitions are underpinned by transient states with surface charge variations, as confirmed by Zeta potential measurements. The accumulated surface charge increases repulsion within the system and favors sliding. Upon cessation of illumination, the system returns to its prior equilibrium state. These findings impact not only nanotribology but nanofluidics and nanorheology. Furthermore, the results underscore the need to consider light-induced effects in other scenarios, including the calculation of activity coefficients of photoactive suspensions. This multifaceted study introduces a new dimension to in operando frictional tuning, beckoning a myriad of applications and fundamental insights at the nanoscale.

[P138-2024] “Influence of the base pressure in deposition of a-SiC<sub>x</sub> interlayers for adhesion of Diamond-Like Carbon on metallic alloy”

Weber, J. S.; Goldbeck, M. C.; Piroli, V.; Boeira, C. D.\*; Perotti, B. L.; Fukumasu, N. K.; Alvarez, F.\*; Michels, A. F.; Figueroa, C. A.

Diamond-like carbon (DLC) is an amorphous material widely used in industrial applications due to its chemical, mechanical, and tribological properties and, also, for decorative purposes. However, its low adhesion to ferrous alloys reduces its effectiveness in certain applications, necessitating the use of adhesion interlayers to reduce stresses at the interfaces and enhance the density of strong bonds. In this context, the factors that promote good adhesion in this system and specify the parameters must be understood in detail. Thus, the present study aims to assess the influence of the base pressure on the deposition of an amorphous silicon carbide adhesion interlayer between DLC coating and a ferrous alloy substrate. Microstructural, physicochemical, morphological, and mechanotribological analyses were conducted to understand the adhesion behavior in terms of structural and chemical aspects. In addition to the influence of the interlayer thickness, the elemental Si/C ratios and the relative oxygen content have an impact on the maximum load supported by the coatings, as well as the different delamination mechanisms generated in adhesion tests.

**SURFACE AND INTERFACE ANALYSIS**, Early Access Date: JUL 2024. DOI: 10.1002/sia.7345

[P139-2024] “Investigation of the stability of metallic grids for large-area perovskite solar cells”

Silva Filho, J. M. C.\*; Morais, A. de\*; Cesar, R. R.; Joanni, E.; Teixeira, R. C.; Marques, F. C.\*; Freitas, J. N. de

Metal contacts are an extremely important part of photovoltaic devices, since they might decrease device stability, or underperform in their function of current extraction. In the case of perovskite solar cells, the metallic component has been less investigated than other cell components, either in the back (rear) contact, or in the form of grid collectors in the front contact. The interaction between the perovskite layer and the metal contact is of utmost importance, since it has been demonstrated for gold and silver (most used metals in perovskite cells) that degradation processes might derive from unwanted contacts between the metal and the perovskite components. Herein, we present a systematic investigation of a series of metals typically used in the electronic or photovoltaic industries (Ag, Al, Au, Cu, Mo, Ni, Pd, Pt, and Ta) in order to assess their stability towards the processing steps of a typical perovskite cell assembly, and also when direct contact between the perovskite and the metal layer takes place. By assessing the morphological and electrical properties of the metal layer after performing a variety of tests, we observed that only four of those metals maintained their integrity. Based on the results, we point out which metal is expected to be most suitable one, from an industrial point of view, and to enable long-term device operation.

**SOLAR ENERGY MATERIALS AND SOLAR CELLS** 276, 113043, 2024. DOI: 10.1016/j.solmat.2024.113043

[P140-2024] “ $K^*(892)_{\pm}$  resonance production in Pb-Pb collisions at  $\sqrt{s_{NN}}=5.02$  TeV”

Acharya, S.; Adamová, D.; Chinellato, D. D.\*; Guardiano, G. G.\*; Jahnke, C.\*; Liveraro, G. S. S.\*; Takahashi, J.\*; et al. ALICE Collaboration

The production of  $K^*(892)_{\pm}$  meson resonance is measured at midrapidity ( $|y| < 0.5$ ) in Pb-Pb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV using the ALICE detector at the CERN Large Hadron Collider. The resonance is reconstructed via its hadronic decay channel  $K^*(892)_{\pm} \rightarrow K-S(0)\pi_{\pm}$ . The transverse momentum distributions are obtained for various centrality intervals in the  $p(T)$  range of 0.4-16 GeV/c.

Measurements of integrated yields, mean transverse momenta, and particle yield ratios are reported and found to be consistent with previous ALICE measurements for  $K^*(892)_{\pm}$  within uncertainties. The  $p(T)$ -integrated yield ratio  $2 K^*(892)_{\pm} / (K^+ + K^-)$  in central Pb-Pb collisions shows a significant suppression at a level of 9.3 sigma relative to pp collisions. Thermal model calculations result in an overprediction of the particle yield ratio. Although both hadron resonance gas in partial chemical equilibrium (HRG-PCE) and MUSIC + SMASH simulations consider the hadronic phase, only HRG-PCE accurately represents the measurements, whereas MUSIC + SMASH simulations tend to overpredict the particle yield ratio. These observations, along with the kinetic freeze-out temperatures extracted from the yields measured for light-flavored hadrons using the HRG-PCE model, indicate a finite hadronic phase lifetime, which decreases with increasing collision centrality percentile. The  $p(T)$ -differential yield ratios  $2 K^*(892)_{\pm} / (K^+ + K^-)$  and  $2 K^*(892)_{\pm} / (\pi^+ + \pi^-)$  are presented and compared with measurements in pp collisions at  $\sqrt{s} = 5.02$  TeV. Both particle ratios are found to be suppressed by up to a factor of five at  $p(T) < 2.0$  GeV/c in central Pb-Pb collisions and are qualitatively consistent with expectations for rescattering effects in the hadronic phase. The nuclear modification factor ( $R_{AA}$ ) shows a smooth evolution with centrality and is found to be below unity at  $p(T) > 8$  GeV/c, consistent with measurements for other light-flavored hadrons. The smallest values are observed in most central collisions, indicating larger energy loss of partons traversing the dense medium.

**PHYSICAL REVIEW C** 109[4], 044902, 2024. DOI: 10.1103/PhysRevC.109.044902

[P141-2024] “Modification of charged-particle jets in event-shape engineered Pb-Pb collisions at  $\sqrt{s_{NN}}=5.02$  TeV”

Acharya, S.; Adamová, D.; Chinellato, D. D.\*; Guardiano, G. G.\*; Jahnke, C.\*; Liveraro, G. S. S.\*; Takahashi, J.\*; et al. ALICE Collaboration

Charged-particle jet yields have been measured in semicentral Pb-Pb collisions at center-of-mass energy per nucleon-nucleon collision  $\sqrt{s_{NN}} = 5.02$  TeV with the ALICE detector at the LHC. These yields are reported as a function of the jet transverse momentum, and further classified by their angle with respect to the event plane and the event shape, characterized by ellipticity, in an effort to study the path-length dependence of jet quenching. Jets were reconstructed at midrapidity from charged-particle tracks using the anti- $k(T)$  algorithm with resolution parameters  $R = 0.2$  and  $0.4$ , with event-plane angle and event-shape values determined using information from forward scintillating detectors. The results presented in this letter show that, in semicentral Pb-Pb collisions, there is no significant difference between jet yields in predominantly isotropic and elliptical events. However, out-of-plane jets are observed to be more suppressed than in-plane jets. Further, this relative suppression is greater for low transverse momentum ( $< 50$  GeV/c)  $R = 0.2$  jets produced in elliptical events, with out-of-plane to in-plane jet-yield ratios varying up to 5.2 sigma between different event-shape classes. These results agree with previous studies indicating that jets experience azimuthally anisotropic suppression when traversing the QGP medium, and can provide additional constraints on the path-length dependence of jet energy loss.

**PHYSICS LETTERS B** 851, 138584, 2024. DOI: 10.1016/j.physletb.2024.138584

[P142-2024] “Observation of abnormal suppression of  $\phi(980)$  production in p-Pb collisions at  $\sqrt{s_{NN}}=5.02$  TeV”

Acharya, S.; Adamová, D.; Chinellato, D. D.\*; Guardiano, G. G.\*; Jahnke, C.\*; Liveraro, G. S. S.\*; Takahashi, J.\*; et al.

The dependence of  $f(0)(980)$  production on the final-state charged-particle multiplicity in p-Pb collisions at  $\sqrt{s(NN)} = 5.02$  TeV is reported. The production of  $f(0)(980)$  is measured with the ALICE detector via the  $f(0)(980) \rightarrow \pi^+\pi^-$  decay channel in a midrapidity region of  $-0.5 < y < 0$ . Particle yield ratios of  $f(0)(980)$  to  $\pi$  and  $K^*(892)(0)$  are found to be decreasing with increasing charged-particle multiplicity. The magnitude of the suppression of the  $f(0)(980)/\pi$  and  $f(0)(980)/K^*(892)(0)$  yield ratios is found to be dependent on the transverse momentum  $p(T)$ , suggesting different mechanisms responsible for the measured effects. Furthermore, the nuclear modification factor  $Q(pPb)$  of  $f(0)(980)$  is measured in various multiplicity ranges. The  $Q(pPb)$  shows a strong suppression of the  $f(0)(980)$  production in the  $p(T)$  region up to about 4 GeV/c. The results on the particle yield ratios and  $Q(pPb)$  for  $f(0)(980)$  may help to understand the late hadronic phase in p-Pb collisions and the nature of the internal structure of  $f(0)(980)$  particle.

PHYSICS LETTERS B 853, 138665, 2024. DOI: 10.1016/j.physletb.2024.138665

[P143-2024] "On the mechanical, thermoelectric, and excitonic properties of Tetragraphene monolayer"

Tromer, R. M.\*; Ribeiro Jr., L. A.; Galvao, D. S.\*; Dias, A. C.; Moujaes, E. A.

Two-dimensional carbon allotropes have attracted much attention due to their extraordinary optoelectronic and mechanical properties, which can be exploited for energy conversion and storage applications. In this work, we use density functional theory simulations and semi-empirical methods to investigate the mechanical, thermoelectric, and excitonic properties of Tetrahexcarbon (also known as Tetragraphene). This quasi-2D carbon allotrope exhibits a combination of squared and hexagonal rings in a buckled shape. Our findings reveal that tetragraphene is a semiconductor material with a direct electronic bandgap of 2.66 eV. Despite the direct nature of the electronic band structure, this material has an indirect exciton ground state of 2.30 eV, which results in an exciton binding energy of 0.36 eV. At ambient temperature, we obtain that the lattice thermal conductivity ( $\kappa(L)$ ) for tetragraphene is approximately 118 W/mK. Young's modulus and the shear modulus of tetragraphene are almost isotropic, with maximum values of 286.0 N/m and 133.7 N/m, respectively, while exhibiting a very low anisotropic Poisson ratio value of 0.09.

MATERIALS TODAY COMMUNICATIONS 39, 109310, 2024. DOI: 10.1016/j.mtcomm.2024.109310

[P144-2024] "Photoproduction of K+K Pairs in Ultraperipheral Collisions"

Acharya, S.; Adamova, D.; Chinellato, D. D.\*; Guardiano, G. G.\*; Jahnke, C.\*; Liveraro, G. S. S.\*; Takahashi, J.\*; et al. ALICE Collaboration

K+K- pairs may be produced in photonuclear collisions, either from the decays of photoproduced  $\phi(1020)$  mesons or directly as nonresonant K+K- pairs. Measurements of K+K- photoproduction probe the couplings between the  $\phi(1020)$  and charged kaons with photons and nuclear targets. The kaon-proton scattering occurs at energies far above those available elsewhere. We present the first measurement of coherent photoproduction of K+K- pairs on lead ions in ultraperipheral collisions using the ALICE detector, including the first investigation of direct K+K- production. There is significant K+K- production at low transverse momentum, consistent with coherent photoproduction on lead targets. In the mass range  $1.1 < M_{KK} < 1.4$  GeV/c<sup>2</sup> above the  $\phi(1020)$  resonance, for rapidity vertical bar  $y(KK)$  vertical bar  $< 0.8$  and  $p(T, KK) < 0.1$  GeV/c,

the measured coherent photoproduction cross section is  $d\sigma/dy = 3.37 \pm 0.61$  (stat)  $\pm 0.15$  (syst) mb. The center-of-mass energy per nucleon of the photon-nucleus (Pb) system  $W(\gamma Pb, n)$  ranges from 33 to 188 GeV, far higher than previous measurements on heavy-nucleus targets. The cross section is larger than expected for  $\phi(1020)$  photoproduction alone. The mass spectrum is fit to a cocktail consisting of  $\phi(1020)$  decays, direct K+K- photoproduction, and interference between the two. The confidence regions for the amplitude and relative phase angle for direct K+K- photoproduction are presented.

PHYSICAL REVIEW LETTERS 132[22, 222303, 2024. DOI: 10.1103/PhysRevLett.132.222303

[P145-2024] "Photoproduction of QED bound states in future electron-ion colliders"

Francener, R.; Gonçaves, V. P.\*; Moreira, B. D.; Santos, K. A.

In this work we perform an exploratory study of the photoproduction of singlet QED bound states ( $l(-)l(+)$ )<sub>S</sub> in electron-ion collisions at the EIC, EIC and LHeC energies. The total cross-sections, event rates per year and rapidity distributions associated with the parapositronium, paramuonium and paratauonium production are estimated. Moreover, we consider the decay of these states in a two-photon system and implement kinematical cuts on the rapidities and energies of the photons in the final state. We demonstrate the paramuonium can, in principle, be observed for the first time in all these colliders and that the EIC is a potential collider to discover the paratauonium state.

PHYSICS LETTERS B 854, 138753, 2024. DOI: 10.1016/j.physletb.2024.138753

[P146-2024] "Plasmonically Active Atomically Thin Titanium-Based Quasicrystals for Dopamine Sensing"

Mandal, N.; Santos, A. B.; Chakraborty, A.; Sarkar, S.; Rao, R.; Glavin, N. R.; Roy, A. K.; Kochat, V.; Yadav, T. P.; Mukhopadhyay, N. K.; Galvao, D. S.\*; Woellner, C. F.; Tiwary, C. S.

Non-noble nanomaterial-based quasicrystals (QC) are attractive structures due to their potential surface plasmon resonance (SPR) properties and ability to be easily exfoliated into two-dimensional (2D) sheets. Interaction with and sensing of organic molecules are applications where such 2D materials are a viable option due to their large surface area to volume ratio, providing abundant active sites for molecular interactions. In this work, a titanium-based multicomponent alloy (Ti<sub>45</sub>Zr<sub>38</sub>Ni<sub>17</sub>) was exfoliated into a 2D quasicrystal (2D-Ti QC) from its bulk form via liquid-phase exfoliation. Structural and optical experimental techniques were used to characterize the 2D-Ti QC. Its plasmonic nature was verified and demonstrated via the absorbance spectrum, light localization images, and far-field diffraction patterns. Dopamine sensing was demonstrated using the absorbance spectra of optically active 2D-Ti QC. The linear range of detection was obtained as similar to 13-91 nM (200-1400 ppb). Molecular dynamics (MD) simulations of Ti QC were conducted to investigate its structural stability. The interaction between 2D-Ti QC and dopamine was investigated by using DFT simulations. In this way, the potential of 2D-Ti QC to be used as an organic molecule sensor has been experimentally and theoretically demonstrated.

ACS APPLIED NANO MATERIALS, 4c02268 Early Access Date: JUN 2024. DOI: 10.1021/acsnm.

[P147-2024] "Quantum mechanics insights into melatonin and analogs binding to melatonin MT1 and MT2 receptors"



Menezes, G. de L.; Bezerra, K. S.\*; Oliveira, J. I. N.; Araujo, J. F.; Galvao, D. S.\*; Silva, R. A. da; Saivish, M. V.; Fulco, U. L.

Melatonin receptors MT1 and MT2 are G protein-coupled receptors that mediate the effects of melatonin, a hormone involved in circadian rhythms and other physiological functions. Understanding the molecular interactions between these receptors and their ligands is crucial for developing novel therapeutic agents. In this study, we used molecular docking, molecular dynamics simulations, and quantum mechanics calculation to investigate the binding modes and affinities of three ligands: melatonin (MLT), ramelteon (RMT), and 2-phenylmelatonin (2-PMT) with both receptors. Based on the results, we identified key amino acids that contributed to the receptor-ligand interactions, such as Gln181/194, Phe179/192, and Asn162/175, which are conserved in both receptors. Additionally, we described new meaningful interactions with Gly108/Gly121, Val111/Val124, and Val191/Val204. Our results provide insights into receptor-ligand recognition's structural and energetic determinants and suggest potential strategies for designing more optimized molecules. This study enhances our understanding of receptor-ligand interactions and offers implications for future drug development.

SCIENTIFIC REPORTS 14[1], 10922, 2024. DOI: 10.1038/s41598-024-59786-x

[P148-2024] "Sachharomyces Cerevisiae Dry Powder-Mediated Exfoliation of Graphite Chunks into Functionalized Few-Layer Graphene"

Mahle, R.; Suran, S.; Singh, A.; Kumbhakar, P.; Galvao, D. S.\*; Cheela, V. R. S.; Dubey, B.; Nair, R. R.; Tiwary, C. S.; Banerjee, R.

Owing to the active production of metabolites during reproduction and growth, microbial cells have been incessantly explored for their potential in the fabrication and functionalization of inorganic materials. Yeast cells, which are nonpathogenic microbes, exhibit biotransformation reactions and the potential to modify functional groups when grown under fermentative conditions. Here, we attempted to delay graphite chunks into graphene flakes by incubating them with dry *Sachharomyces cerevisiae* powder. The evident delamination/thinning of graphene layers was demonstrated using microscopic and spectroscopic analyses which confirmed the exfoliation of graphite to few-layer graphene (FLG). The gate-to-gate life cycle assessment (LCA) of the developed process established the sustainability and environmental hotspots for the approach. Our study demonstrates the facile, green, and sustainable exfoliation of graphite using off-the-shelf materials in laboratories or kitchens and can be scaled up to industry levels. Yeast cells were also explored for the exfoliation of another 2D material, MoS<sub>2</sub>, and showed the potential to flake off the bulk structure into few MoS<sub>2</sub> sheets.

ACS SUSTAINABLE CHEMISTRY & ENGINEERING, Early Access Date: JUL 2024. DOI: 10.1021/acssuschemeng.4c00832

[P149-2024] "Schwarzites and Triply Periodic Minimal Surfaces: From Pure Topology Mathematics to Macroscale Applications"

Felix, L. C.\*; Ambekar, R.; Tromer, R. M.\*; Woellner, C. F.; Rodrigues, V.\*; Ajayan, P. M.; Tiwary, C. S.; Galvao, D. S.\*

Schwarzites are porous (spongy-like) carbon allotropes with negative Gaussian curvatures. They are proposed by Mackay and Terrones inspired by the works of the German mathematician Hermann Schwarz on Triply-Periodic Minimal Surfaces (TPMS). This review presents and discusses the history of schwarzites and their place among curved carbon nanomaterials. The main works on schwarzites are summarized and are available in the literature.

Their unique structural, electronic, thermal, and mechanical properties are discussed. Although the synthesis of carbon-based schwarzites remains elusive, recent advances in the synthesis of zeolite-templates nanomaterials have brought them closer to reality. Atomic-based models of schwarzites are translated into macroscale ones that are 3D-printed. These 3D-printed models are exploited in many real-world applications, including water remediation and biomedical ones. Schwarzites are porous (spongy-like) carbon allotropes with negative Gaussian curvatures. They are proposed by Mackay and Terrones inspired by the works of the German mathematician Hermann Schwarz on Triply-Periodic Minimal Surfaces (TPMS). This review presents and discusses the history of schwarzites and their place among curved carbon nanomaterials.

SMALL, Early Access Date: JUN 2024. DOI: 10.1002/sml.202400351

[P150-2024] "Search for pair production of scalar and vector leptosquarks decaying to muons and bottom quarks in proton-proton collisions at  $\sqrt{s}=13$  TeV"

Hayrapetyan, A.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; et al.  
CMS Collaboration

A search for pair production of scalar and vector leptosquarks (LQs) each decaying to a muon and a bottom quark is performed using proton-proton collision data collected at root  $s = 13$  TeV with the CMS detector at the CERN LHC, corresponding to an integrated luminosity of 138 fb<sup>-1</sup>. No excess above standard model expectation is observed. Scalar (vector) LQs with masses less than 1810 (2120) GeV are excluded at 95% confidence level, assuming a 100% branching fraction of the LQ decaying to a muon and a bottom quark. These limits represent the most stringent to date.

PHYSICAL REVIEW D 109[11], 112003, 2024. DOI: 10.1103/PhysRevD.109.112003

[P151-2024] "Signal, detection and estimation using a hybrid quantum circuit"

Sá Neto, O. P. de; Oliveira, M. C. de\*

We investigate a hybrid device allowing a photon-phonon coupling of a transmission line radiation (TLR) and a nanoelectromechanical system (NEMS), mediated by a superconducting qubit population imbalance. We demonstrate the derivation of an effective Hamiltonian for the strongly dispersive regime for this system. The qubit works as a quantum switch, allowing a conditioned transfer of excitations between the TLR and NEMS. We show that this regime allows the system to be employed for signal processing and force estimation. Additionally, we explore the ability of the quantum switch to generate non-classical states.

SCIENTIFIC REPORTS 14[1], 15225, 2024. DOI: 10.1038/s41598-024-65520-4

[P152-2024] "Solid-State NMR Characterization of Mefloquine Resinate Complexes Designed for Taste-Masking Pediatric Formulations"

Borré, L. B.; Sousa, E. G. R.; San Gil, R. A. S.; Baptista, M. M.; Leitao, A. A.; Almeida, Joao M. A. R. de; Carr, O.; Oliveira Jr., O. N.; Shimizu, F. M.\*; Guimaraes, T. F.

Mefloquine (MQ) is an antimalarial medication prescribed to treat or malaria prevention. When taken by children, vomiting usually occurs, and new doses of medication frequently need to be taken.

So, developing pediatric medicines using taste-masked anti-malarial drug complexes is mandatory for the success of mefloquine administration. The hypothesis that binding mefloquine to an ion-exchange resin (R) could circumvent the drug's bitter taste problem was proposed, and solid-state C-13 cross-polarization magic angle spinning (CPMAS) NMR was able to follow MQ-R mixtures through chemical shift and relaxation measurements. The nature of MQ-R complex formation could then be determined. Impedimetric electronic tongue equipment also verified the resin's taste-masking efficiency in vitro. Variations in chemical shifts and structure dynamics measured by proton relaxation properties (e.g., T1 rho(H)) were used as probes to follow the extension of mixing and specific interactions that would be present in MQ-R. A significant decrease in T1 rho(H) values was observed for MQ carbons in MQ-R complexes, compared to the ones in MQ (from 100-200 ms in MQ to 20-50 ms in an MQ-R complex). The results evidenced that the cationic resin interacts strongly with mefloquine molecules in the formulation of a 1:1 ratio complex. Thus, C-13 CPMAS NMR allowed the confirmation of the presence of a binding between mefloquine and polacrilin in the MQ-R formulation studied.

**PHARMACEUTICALS 17[7], 870, 2024. DOI: 10.3390/ph17070870**

**[P153-2024] "Structural and Magnetic Transformations from CuCl to Cu2Cl(OH)3 Induced by H2O and CuCl2"**

**Pimentel, D. P.\***

This study explores the oxidation dynamics of "pure" CuCl during prolonged environmental exposure through X-ray diffraction and temperature-dependent magnetization assessments. While CuCl is traditionally considered diamagnetic, our investigation reveals the emergence of an antiferromagnetic transition at 4.7 K. This anomaly is potentially induced by the integration of water molecules into the CuCl matrix. The hydration process initiates a series of oxidation reactions, ultimately transmuting CuCl into Cu2Cl(OH)3. Over time, the distinctive diffractogram peaks corresponding to CuCl diminish, concurrently with the appearance and intensification of those ascribed to Cu2Cl(OH)3, culminating in a complete phase transition as confirmed by X-ray analysis. Correspondingly, magnetization measurements clearly discern magnetic transitions at 6.4 and 16 K, intensifying with the sample's exposure duration. These findings illuminate the stark potential for probing the magnetic intricacies of Cu2Cl(OH)3, a subject that remains a compelling and unresolved intrigue within the field.

**JETP LETTERS, Early Access Date: JUN 2024. DOI: 10.1134/S0021364024601763**

**[P154-2024] "Study of long term stability of a 50 liters TPC, based on TRIPLE-GEM with optical readout, for the CYGNO experiment"**

**Amaro, F. D.; Antonietti, R.; Baracchini, E.; Kemp, E.\*; et al.**

The CYGNO project aims to study rare events, as low -mass (few GeV) Dark Matter (DM) particle or solar neutrino interactions, exploiting the approach of the optical readout of the scintillation light produced in the amplification in a multiple Gas Electron Multiplier (GEM) structure, of the primary ionization originated in large volume Time Projection Chamber (TPCs). The volume is filled with an He:CF 4 gas mixture at atmospheric pressure. The 3D topology, and therefore direction of the recoils, is reconstructed thanks to the combined use of high -granularity, high sensitivity sCMOS cameras, for the precise tracking of the projection of the recoils on the GEM plane, and of fast light sensors in order to obtain the coordinate perpendicular to the camera plane.

To conclude the R&D phase, the 50 L prototype, called Long Imaging ModuLE (LIME), was moved underground at the Laboratori Nazionali del Gran Sasso (LNGS) in order to study the performance of the CYGNO experimental approach in a low background environment and to assess the contributions to the background from different sources, also comparing with Monte Carlo simulations. Stability studies and the effects of environmental condition on the light yield will be discussed, focusing on the effect of humidity on the detector response and stability amount and rate of self-sustaining micro -discharges. This is a crucial step towards the development of a large demonstrator.

**NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT 1065, 169473, 2024. DOI: 10.1016/j.nima.2024.169473**

**[P155-2024] "The physics of ultra-high-energy cosmic rays in the context of the Pierre Auger Observatory: Main results and future perspectives"**

**Anastasi, G. A.; Arbeletche, L. B.\*; Chinellato, J. A.\*; Franco, D de O.\*; Dobrigkeit, C.\*; Fauth, A. C.\*; Payeras, A. M.\*; et al.  
Pierre Auger Collaboration**

For almost 20 years, the Pierre Auger Observatory has studied ultrahigh -energy cosmic rays (UHECRs) using its unique hybrid design, which employs a ground array of water -Cherenkov detectors along with 27 fluorescence telescopes to observe extensive air showers with different, complementary techniques. Some fundamental results include measurements of the energy spectrum, of the primary mass composition and of the arrival directions with unprecedented accuracy. Although no specific source has been pinpointed yet, these findings have significantly improved our understanding of UHECR and set the stage for the upgrade of the experimental setup, called AugerPrime, currently under finalization.

**NUOVO CIMENTO C-COLLOQUIA AND COMMUNICATIONS IN PHYSICS 47[3], 65, 2024. DOI: 10.1393/ncc/i2024-24065-4**

**[P156-2024] "Thickness dependent nanoscale magnetism in two-dimensional manganese telluride (MnTe)"**

**Slathia, S.; Tripathi, M.; Tromer, R.\*; Gowda, C. C.; Pandey, P.; Galvao, D. S.\*; Dalton, A.; Tiwary, C. S.**

Magnetism from two-dimensional (2D) materials has received significant attention and admiration due to their unique electronic and magnetic properties owing to quantum confinement, such as spin-orbit coupling, magnetic anisotropy, and emergent magnetic orders, leading to behaviors and properties not observed in bulk materials. One of the crucial gaps that need to be addressed is deciphering the ordering of magnetic behavior with the thickness of manganese dichalcogenides, manganese telluride (MnTe). The present work explores the pivotal role of thickness in modulating the magnetic properties of 2D MnTe, obtained using liquid-phase exfoliation techniques. Intriguing magnetic and electronic properties have been observed in MnTe thinner than 5 nm. Our experimental findings and density functional theory (DFT) calculations revealed the transition from antiferromagnetic characteristics to ferromagnetic behavior for one to two layers and then back to antiferromagnetic behavior for thicknesses larger than 5 nm. These results demonstrate the existence of thickness-dependent transitions in magnetic ordering and anisotropy for the 2D materials. The experimental results, in conjunction with theoretical modeling, unravel useful insights into the implications of magnetic 2D MnTe for emerging technologies driven by nanoscale magnetism, such as spintronics and quantum computing.

The outcomes from the present work open new possibilities for developing memory devices with enhanced functionality and efficiency.

**MATERIALS TODAY CHEMISTRY 38, 102134, 2024. DOI: 10.1016/j.mtchem.2024.102134**

**[P157-2024] “Unveiling Challenging Microbial Fossil Biosignatures from Rio Tinto with Micro-to-Nanoscale Chemical and Ultrastructural Imaging”**

Maldanis, L.; Fernandez-Remolar, D.; Lemelle, L.; Knoll, A. H.; Guizar-Sicairos, M.; Holler, M.; Silva, F. M. C. da\*; Magnin, V.; Mermoux, M.; Simionovici, A.

Understanding the nature and preservation of microbial traces in extreme environments is crucial for reconstructing Earth's early biosphere and for the search for life on other planets or moons. At Rio Tinto, southwestern Spain, ferric oxide and sulfate deposits similar to those discovered at Meridiani Planum, Mars, entomb a diversity of fossilized organisms, despite chemical conditions commonly thought to be challenging for life and fossil preservation. Investigating this unique fossil microbiota can elucidate ancient extremophile communities and the preservation of biosignatures in acidic environments on Earth and, potentially, Mars. In this study, we use an innovative multiscale approach that combines the state-of-the-art synchrotron X-ray nanoimaging methods of ptychographic X-ray computed laminography and nano-X-ray fluorescence to reveal Rio Tinto's microfossils at subcellular resolution. The unprecedented nanoscale views of several different specimens within their geological and geochemical contexts reveal novel intricacies of preserved microbial communities. Different morphotypes, ecological interactions, and possible taxonomic affinities were inferred based on qualitative and quantitative 3D ultrastructural information, whereas diagenetic processes and metabolic affinities were inferred from complementary chemical information. Our integrated nano-to-microscale analytical approach revealed previously invisible microbial and mineral interactions, which complemented and filled a gap of spatial resolution in conventional methods. Ultimately, this study contributes to the challenge of deciphering the faint chemical and morphological biosignatures that can indicate life's presence on the early Earth and on distant worlds.

**ASTROBIOLOGY 24[7], 721-733, 2024. DOI: 10.1089/ast.2023.0127**

**[P158-2024] “Valence instability and collapse of ferromagnetism in EuB<sub>6</sub> at high pressures”**

Kutelak, L. O.\*; Sereika, R.; Fabbris, G.; Francisco, L.\*; Lombardi, G.\*; Poldi, E. H. T.\*; Zhao, J.; Alp, E. E.; Souza Neto, N. M.; Rosa, P. F. S.; Haskel, D.; Bi, W.; Reis, R. D. dos

Despite the simplicity of their cubic crystal lattice, rare-earth hexaborides display complex physical properties including a (long debated) onset of metallization via magnetic polaron formation at Tc1 approximate to 15 K preceding ferromagnetic ordering at Tc2 approximate to 12 K. In this work, we used applied pressure to tune the interplay between electronic structure and magnetism in EuB<sub>6</sub>. We probed the magnetism, valence, and structure of EuB<sub>6</sub> under quasi-hydrostatic pressures up to 30 GPa using X-ray techniques. Our findings show evidence for collapse of ferromagnetism above 20 GPa following a monotonic increase of mean Eu valence. While X-ray diffraction measurements in the paramagnetic state at room temperature show that the lattice retains cubic symmetry, a measurable quadrupole interaction seen by time-domain synchrotron M & ouml;ssbauer spectroscopy suggests a lowering of symmetry associated with magnetic ordering, becoming more prominent across the magnetic transition.

The interplay between conduction band electron count and magnetism observed under applied pressure in EuB<sub>6</sub> opens possibilities for fine-tuning metallization and magnetic properties of similar Eu-based semi-metal systems.

**JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS 603, 172203, 2024. DOI: 10.1016/j.jmmm.2024.172203**

**[P159-2024] “X-ray dose effects and strategies to mitigate beam damage in metal halide perovskites under high brilliance X-ray photon sources”**

Silva, F. M. C. da\*; Szostak, R.; Guaita, M. G. D.; Teixeira, V. C.; Nogueira, A. F.; Tolentino, H. C. N.

Metal halide perovskites (MHP) suffer from photo-structural-chemical instabilities whose intricacy requires state-of-the-art tools to investigate their properties under various conditions. This study addresses the damage caused by focused X-ray beams on MHP through a correlative multi-technique approach. The damage after high-dose irradiation is noticeable in many ways: the loss of iodine and organic components, whose relative amount is reduced; the formation of an excavated area modifying the sample morphology; and an altered optical reflectivity indicating an optically inactive layer. The damage mechanism combines radiolysis and sputtering processes. Interestingly, the bulk underneath the excavated area maintains the initial halide proportion demonstrated by a stable photoluminescence emission energy. We also show that controlling the beam dose and environment is an excellent strategy to mitigate the dose harm. Hence, we combined a controlled X-ray dose with an inert N<sub>2</sub> atmosphere to certify the conditions to probe MHP properties while mitigating damage efficiently. Finally, we applied optimized conditions in an X-ray ptychography experiment, reaching a 15-nm spatial resolution, an outcome that has never been attained in this class of materials.

**ENERGY MATERIALS 4[5], 400058, 2024. DOI: 10.20517/energymater.2023.114**

**\*Autores da comunidade IFGW**  
Fonte: Web of Science on-line (WOS)

## Defesas de Dissertações do IFGW

**[D016-2024] “Dois problemas em populações: especiação e auto-organização”**

Aluno: Joao Ulises Fabián Lizárraga  
Orientador: Prof. Dr. Marcos Aloizio Martinez de Aguiar  
Data: 29/07/2024

**[D017-2024] “Redes em Desenvolvimento em Diferentes Escalas”**

Aluno: Maria Gabriela Magalhães Veloso  
Orientador: Prof. Dr. José Antônio Brum  
Data: 08/08/2024

**[D018-2024] “Desenvolvimento de Técnicas para Design de Amplificadores Paramétricos Modulados Por Fluxo e Baseados em Junções Josephson”**

Aluno: Diego Molina Sanches Silva  
Orientador: Prof. Dr. Francisco Paulo Marques Rouxinol  
Data: 15/08/2024

[D019-2024] “Integração híbrida com fotônica de silício”  
Aluno: Maria Carolina França Volpato  
Orientador: Prof. Dr. Newton Cesário Frateschi  
Data: 23/08/2024

## Defesas de Teses do IFGW

[T011-2024] “Explorando Efeitos de Interface e Defeitos Pontuais em Heteroestruturas de Materiais 2D: Um Estudo sobre TMDCs e h-BN”

Aluno: Fábio Juvêncio Ramalho Costa  
Orientador: Prof. Dr. Luiz Fernando Zagonel  
Data: 23/08/2024

[T012-2024] “Abordagem de deep learning para sistemas quânticos de muitos corpos”

Aluno: William Freitas e Silva  
Orientador: Prof. Dr. Silvio Antonio Sachetto Vitiello  
Data: 30/08/2024

Fonte: Portal IFGW/Eventos

Disponível em: <https://portal.ifi.unicamp.br/a-instituicao/eventos/month.calendar/2023/12/14/>

## Defesas de Dissertações e Teses do PECIM

[P006-2024] “O currículo e a formação inicial de professores de física para o uso de tecnologias digitais de informação e comunicação: um olhar sobre as licenciaturas das universidades estaduais paulistas”

Aluno: Eugenio Rodrigues Rosa do Nascimento  
Orientador: Prof. Dr. Guilherme Stecca Marcom  
Banca: Prof. Dr. Guilherme Stecca Marcom - Orientador, Profa. Dra. Juliana Rink - FE/ UNICAMP, Prof. Dr. Marcelo Alves Barros/ UNICAMP, Prof. Dr. Juliano Camillo - FE / Unicamp - suplente, Prof. Dr. Sandro Guedes de Oliveira/suplente

Data: 28/06/2024

Exame de Defesa: Mestrado

[P007-2024] “Os percursos neoliberais por meio dos itinerários formativos no currículo paulista - reflexões sobre o novo ensino médio”

Aluno: Erica Cristina Frau  
Orientador: Prof. Dr. Fernando Santiago dos Santos  
Banca: Prof. Dr. Fernando Santiago dos Santos - orient. / Presidente, Profa. Dra. Nora Rut Krawczyk - titular, Prof. Dr. Guilherme Stecca Marcom - titular, Profa. Dra. Ivana Elena Camejo Aviles - suplente, Prof. Dr. Fernando Rogério da Cruz - suplente

Data: 27/08/2024

Exame de Defesa: Doutorado

Fonte: Página do PECIM

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## Abstracta

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