

Abstracta

Ano XXIX - N. 06

Dez-25



INSTITUTO DE FÍSICA
GLEB WATAGHIN



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Novidade: agora os trabalhos possuem os links para o texto publicado nas revistas.

Artigos publicados

[P304-2025] “A Hybrid All-Solid-State Supercapacitor Using a Dry Multilayered Graphene Oxide Electrolyte Assembly: Understanding the Charging Dynamics from Experimental and Molecular Simulation Studies”

Jimenez, M. J. M.*; Maria, M. A. E.*; Leidens, L. M.*; Fonseca, A. F.*; Silva, M. A. P. da; Rodrigues, V.*; Alvarez, F.*; Riul Jr., A.*

Research in supercapacitors is essential for driving innovation in energy storage, paving the way for a more sustainable and efficient future where technology and the environment coexist in harmony. Supercapacitors can instantly provide higher energy density than conventional capacitors and higher power density than batteries, despite limitations of low volumetric performance. Here, we show a simplified way to manufacture a hybrid all-solid-state supercapacitor operating at room temperature and dry conditions based on poly(diallyldimethylammonium chloride) (PDDA)/graphene oxide (GO) multilayer assembly using the layer-by-layer technique. They display rapid discharge (relaxation time constant, τ_0 down to 1 μ s), high energy (up to 7 Wh/kg) and power (up to 1400 W/kg) densities, and specific capacitance (up to 12 F/g). Molecular dynamics simulations of a PDDA/GO system are performed with and without water molecules, highlighting the crucial role of chlorine in the system's structure. The charge storage and fast discharge, LbL thickness control, and film conformability on practically any surface are attractive approaches in numerous practical applications. Besides simplifying the system, the exclusion of liquid electrolytes and the use of ultrathin films are advantageous in several applications, without compromising weight in structures.

ACS OMEGA 10[42], p. 50611-50625, 2025. DOI: 10.1021/acsomega.5c00990. Acesso: <https://doi.org/10.1021/acsomega.5c00990>

[P305-2025] “A planar T-carbon structure with tunable electric and optical properties via chemical decorations on the (111) plane: a first-principles investigation”

Cai, H. F.; Duan, Z. W.; Cai, K.; Galvao, D. S.*; Qin, Q. H.

We proposed a novel two-dimensional carbon allotrope designated as 2-(111) planar T-carbon, obtained by slicing bulk T-carbon along its (111) crystallographic direction. This orientation selection is rationalized by two critical factors: the (111) surface exhibits the most intense diffraction signature in experimental characterization and demonstrates the lowest surface energy among potential cleavage planes. Through systematic first-principles investigations, we demonstrate that surface chemical decoration serves as an effective strategy to simultaneously engineer the optoelectronic characteristics and enhance the thermal/dynamic stability of 2-(111) planar T-carbon. Comparative analysis of DFT-calculated phonon spectra between pristine and three decorated configurations confirms that surface functionalization provides a promising and feasible pathway to achieve structural stabilization. First-principles calculations reveal a tunable direct bandgap ranging from 0.81 eV (-OH decorated) to 2.81 eV (hydrogenated), with chemical modifications inducing predictable blue shifts in optical spectra. Furthermore, the simultaneous application of multiple chemical decorations enables progressive tuning of optoelectronic properties, establishing a gradient modulation platform for performance optimization.

MATERIALS ADVANCES, 2025. DOI: 10.1039/d5ma00578g Early Access Date: OCT 2025. Acesso: <https://doi.org/10.1039/d5ma00578g>

[P306-2025] “Abnormal crack coalescence and ductility in graphene”

Jin, S.; Hong, J. W.; Daraio, C.; Fonseca, A. F.*

Crack coalescence is a critical component in the study of mechanical resistance and the stability of materials. In the particular case of graphene, despite the extensive investigation of the formation and behavior of individual cracks in graphene, the study of crack coalescence within its structure remains unexplored. In this study, we investigate the interaction between two pre-existing cracks and their effect on the mechanical properties of graphene using molecular dynamics simulations. The behavior of zigzag and armchair graphene structures with cracks separated by distances (W_{gap}) is analyzed under tensile loading. The findings reveal that crack coalescence, defined as the formation of a new crack from two existing crack tips, occurs for lower values of the distance between cracks, W_{gap} , resulting in a decline in the strength of structures. As W_{gap} increases, the stress-strain curves shift upward, with the peak stress rising in the absence of crack coalescence. The effective stress intensity factor formulated in this study exhibits a clear upward trend with increasing W_{gap} . Furthermore, an increase in W_{gap} induces a transition in fracture behavior from crack coalescence to independent propagation with intercrack undulation. This shift in fracture behavior demonstrates a brittle-to-ductile transition, as evidenced by increased energy absorption and delayed failure. A design guideline for the initial crack geometry is suggested by correlating peak stress with W_{gap} , within a certain range. The findings offer insights into the fracture mechanics of graphene, emphasizing the impact of crack interaction and geometry on strength. This provides design guidelines for graphene-based structures with enhanced mechanical performance.

INTERNATIONAL JOURNAL OF MECHANICAL SCIENCES 309, 111025, 2025, DOI: 10.1016/j.ijmecsci.2025.111025. Acesso: <https://doi.org/10.1016/j.ijmecsci.2025.111025>

[P307-2025] “Accelerating feedback-based quantum algorithms through time rescaling”

Rattighieri, L. A. M.*; Peixe, G. E. L.; Bernardo, B. L.; Fanchini, F. F.

This work investigates the impact of time rescaling on the performance of Feedback-Based Quantum Algorithms (FQAs) and their variant for optimization tasks, Feedback-Based Algorithm for Quantum Optimization (FALQON). We introduce the Time-Rescaled Feedback-Based Quantum Algorithm (TR-FQA) and TimeRescaled Feedback-Based Algorithm for Quantum Optimization (TR-FALQON), time-rescaled versions of FQA and FALQON, respectively. The method is applied to two representative problems: the MaxCut combinatorial optimization problem and ground-state preparation in the axial next-nearest neighbor Ising (ANNNI) model. The results show that TR-FALQON accelerates convergence toward the optimal solution in the circuit's early layers and outperforms the standard version in low-depth regimes. In the context of state preparation, TR-FQA requires fewer layers than the original algorithm. These findings suggest that time rescaling can reduce the number of layers needed to reach a high-quality solution, even if the exact ground state is not obtained.

PHYSICAL REVIEW A 112[4], 042607, 2025. DOI: 10.1103/physreva.112.042607. Acesso: <https://doi.org/10.1103/physreva.112.042607>

[P308-2025] “Alleviating the present tension between T2K and NOvA with nonstandard neutrino interactions”

Cherchiglia, A.*; Pasquini, P.*; Peres, O. L. G.*; Rodrigues, F. F.*; Rossi, R. R.*; Souza, E. S.*

Since neutrino oscillation was observed, several experiments have been built to measure its parameters. NuMI Off-axis ν_e Appearance (NO ν A) and Tokai-to-Kamioka (T2K) are two long-baseline experiments dedicated to measuring mainly the mixing angle θ_{23} , the charge-parity (CP) conjugation phase δ_{CP} , and the mass ordering. However, there is a tension in current data. The T2K allowed region is in conflict with the region allowed by NO ν A. We propose a nonstandard charged current interaction (CC-NSI) in neutrino production to relieve this tension. The CC-NSI is computed through quantum field theory formalism, where we derive perturbative analytical formulae considering CC-NSI in the pion decay. Within this new approach, we can alleviate NO ν A and T2K tension for CC-NSI complex parameters of order 10^{-3} . We show the new phase has a degeneracy to the Dirac CP phase of the form $\delta_{CP} + \pi = 1.52c$, being a possible source of violation of charge-parity symmetry.

PHYSICAL REVIEW D 112[9], 093004, 2025. DOI: 10.1103/55qm-zbhv. Acesso: <https://doi.org/10.1103/55qm-zbhv>

[P309-2025] “Angular analysis of the $B^0 \rightarrow K^*(892)0\mu^+\mu^-$ decay in proton-proton collisions at $\sqrt{s}=13$ TeV”

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

A full set of optimized observables is measured in an angular analysis of the decay $B^0 \rightarrow K^*(892)0\mu^+\mu^-$ using a sample of proton-proton collisions at $\sqrt{s} = 13$ TeV, collected with the CMS detector at the LHC, corresponding to an integrated luminosity of 140 fb $^{-1}$. The analysis is performed in six bins of the squared invariant mass of the dimuon system, q^2 , over the range $1.1 < q^2 < 16$ GeV 2 . The results are among the most precise experimental measurements of the angular observables for this decay and are compared to a variety of predictions based on the standard model. Some of these predictions exhibit tension with the measurements.

PHYSICS LETTERS B 864, 139406, 2025. DOI: 10.1016/j.physletb.2025.139406. Acesso: <https://doi.org/10.1016/j.physletb.2025.139406>

[P310-2025] “Bayesian network 3D event reconstruction in the Cygno optical TPC for dark matter direct detection”

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

The CYGNO experiment is developing a high-resolution gaseous Time Projection Chamber with optical readout for directional dark matter searches. The detector uses a helium-tetrafluoromethane (He:CF $_4$ 60:40) gas mixture at atmospheric pressure and a triple Gas Electron Multiplier amplification stage, coupled with a scientific camera for high-resolution 2D imaging and fast photomultipliers for time-resolved scintillation light detection. This setup enables 3D event reconstruction: photomultiplier signals provide depth information, while the camera delivers high-precision transverse resolution. In this work, we present a Bayesian Network-based algorithm designed to reconstruct the events using only the photomultiplier signals, inferring a 3D description of the particle trajectories. The algorithm models the light collection process probabilistically and estimates spatial and intensity parameters on the Gas Electron Multiplier plane, where light emission occurs. It is implemented within the Bayesian Analysis Toolkit and uses Markov Chain Monte Carlo sampling for posterior inference. Validation using data from the CYGNO LIME prototype shows accurate reconstruction of localized and extended straight tracks.

Results demonstrate that the Bayesian approach enables robust 3D description and, when combined with camera data, opens the way to future improvements in spatial and energy resolution. This methodology represents a significant step forward in directional dark matter detection, enhancing the identification of nuclear recoil tracks with high spatial resolution.

EUROPEAN PHYSICAL JOURNAL C 85[11], 1261, 2025. DOI: 10.1140/epjc/s10052-025-14965-6. Acesso: <https://doi.org/10.1140/epjc/s10052-025-14965-6>

[P311-2025] “Brain Functional Connectivity is Altered in Professional Footballers With Previous Hamstring Injury”

Carneiro, P. P.*; Correia, J. P.; Castellano, G.*; Freitas, S. R.

Purpose: To investigate how hamstring injuries affect brain functional connectivity (FC) and identify potential biomarkers for injury assessment and rehabilitation. Methods: Brain activity was recorded during a rigorous motor task using electroencephalography in 129 footballers. Demographic, anthropometric, injury, and football-related data were also collected. Brain FC was calculated separately for the rest and activity periods. A 2-way mixed analysis of variance was conducted for group comparisons, and a partial correlation analysis examined links between FC and injury parameters. Results: The execution of the motor task led to a significant decrease in alpha-band FC during activity compared with rest (injured: $P < .0001$, $\eta^2(p)=.38$; control: $P < .001$, $\eta^2(p)=.11$). Injured players showed significantly lower FC during activity ($P = .006$, $\eta^2 p=.07$), as well as a greater decrease from rest to activity ($P < .001$, $\eta^2(p)=.13$), particularly in the frontal ($P < .001$, $\eta^2(p)=.17$) and temporal ($P = .03$, $\eta^2 p=.08$) regions. There were significant inverse correlations between the injury severity index and global ($P = .003$, $r = -.58$), frontal ($P < .001$, $r = -.72$), and parietal ($P = .015$, $r = -.59$) connectivity. Conclusion: Reduced FC in footballers with previous hamstring injury suggests an increased cognitive effort required for task execution, namely, in regions associated with motor planning and movement sequencing. The correlation analysis results point to a relationship between age and severity of the injury and the degree of this increase in cognitive effort.

INTERNATIONAL JOURNAL OF SPORTS PHYSIOLOGY AND PERFORMANCE, 2025. DOI: 10.1123/ijspp.2024-0559 Early Access Date: OCT 2025. Acesso: <https://doi.org/10.1123/ijspp.2024-0559>

[P312-2025] “Charged-particle multiplicity distributions over a wide pseudorapidity range in p-Pb collisions at $\sqrt{s_{NN}}=5.02$ TeV”

Acharya, S.; Agarwal, A.; Rinella, G. A.; Jahnke, C.*; Liveraro, G. S. S.*; Takahashi, J.*; et al.
ALICE Collaboration

This paper presents the primary charged-particle multiplicity distributions in proton-lead collisions at a centre-of-mass energy per nucleon-nucleon collision of $\sqrt{s_{NN}} = 5.02$ TeV. The distributions are reported for non-single diffractive collisions in different pseudorapidity ranges. The measurements are performed using the combined information from the Silicon Pixel Detector and the Forward Multiplicity Detector of ALICE. The multiplicity distributions are parametrised with a double negative binomial distribution which provides satisfactory descriptions of the distributions for all the studied pseudorapidity intervals. The data are compared to models and analysed quantitatively, evaluating the first four moments (mean, standard deviation, skewness, and kurtosis).

The shape evolution of the measured multiplicity distributions is studied in terms of KNO variables and it is found that none of the considered models reproduces the measurements. This paper also reports on the average charged-particle multiplicity, normalised by the average number of participating nucleon pairs, as a function of the collision energy. The multiplicity results are then compared to measurements made in proton-proton and nucleus-nucleus collisions across a wide range of collision energies.

EUROPEAN PHYSICAL JOURNAL C 85[8], 919, 2025. DOI: 10.1140/epjc/s10052-025-14577-0. Acesso: <https://doi.org/10.1140/epjc/s10052-025-14577-0>

[P313-2025] “Constraints on Energy Scales from Dark Matter Decay in a Gauged B - L Model”

Gambini, G.; Holanda, P. C. de*; Carneiro, S.

Popular extensions of the standard model of particle physics feature new fields and symmetries which could, for example, dynamically generate neutrino masses from B - L spontaneous symmetry breaking. If a new light scalar that decays into dark radiation appears in the spectrum of the theory, it could significantly modify the cosmological observables. In this case, cold dark matter could have a stable and a decaying component and limits on its decay rate Γ_{dcdm} can be used to put constraints on the new energy scales of a given model. We illustrate this idea using a gauged B - L model where the dark radiation is in the form of light neutrinos.

BRAZILIAN JOURNAL OF PHYSICS 56[1], 30, 2025. DOI: 10.1007/s13538-025-01952-1. Acesso: <https://doi.org/10.1007/s13538-025-01952-1>

[P314-2025] “Constraints on standard model effective field theory for a Higgs boson produced in association with W or Z bosons in the $H \rightarrow b\bar{b}$ decay channel in proton-proton collisions at $\sqrt{s}=13$ TeV”

Chekhovsky, V.; Hayrapetyan, A.; Chinellato, J. A.*; et al. CMS Collaboration

A standard model effective field theory (SMEFT) analysis with dimension-six operators probing nonresonant new physics effects is performed in the Higgs-strahlung process, where the Higgs boson is produced in association with a W or Z boson, in proton-proton collisions at a center-of-mass energy of 13 TeV. The final states in which the W or Z boson decays leptonically and the Higgs boson decays to a pair of bottom quarks are considered. The analyzed data were collected by the CMS experiment between 2016 and 2018 and correspond to an integrated luminosity of 138 fb⁻¹. An approach designed to simultaneously optimize the sensitivity to Wilson coefficients of multiple SMEFT operators is employed. Likelihood scans as functions of the Wilson coefficients that carry SMEFT sensitivity in this final state are performed for different expansions in SMEFT. The results are consistent with the predictions of the standard model.

JOURNAL OF HIGH ENERGY PHYSICS [3], 114, 2025. DOI: 10.1007/JHEP03(2025)114. Acesso: [https://doi.org/10.1007/JHEP03\(2025\)114](https://doi.org/10.1007/JHEP03(2025)114)

[P315-2025] “Diode effect for skyrmions interacting with linear protrusion defects”

Souza, J. C. B.*; Reichhardt, C. J. O.; Reichhardt, C.; Vizirim, N. P.*; Venegas, P. A.

We simulate collectively interacting skyrmions in a channel with periodic asymmetry, and find a strong diode effect for the skyrmion flow.

There is also an asymmetry in the skyrmion annihilation rate for currents applied along the hard or easy substrate asymmetry direction, with a higher annihilation rate for hard direction currents. We map out the diode efficiency as a function of magnetic field and substrate asymmetry angle. We also show that the Magnus force impacts the diode motion and annihilation rate asymmetry by forcing skyrmions into corners of the protrusion geometry.

NEW JOURNAL OF PHYSICS 27[11], 113501, 2025. DOI: 10.1088/1367-2630/ae1637. Acesso: <https://iopscience.iop.org/article/10.1088/1367-2630/ae1637>

[P316-2025] “Effect of tDCS targeting the dorsolateral prefrontal cortex on psychophysiological responses and brain oxygenation during exercise in healthy adults: a proof-of-concept randomized controlled trial”

Machado, D. G. da S.; Melo, M. J. L. de; Mendonça, M. A.; Leiros, D. de M.; Silva, E. B. da; Forti, R. M.*; Mesquita, R. C.*; Faro, H.; Acevedo, E. O.

Background: Physical inactivity is a major public health challenge, and strategies to improve exercise adherence are crucial. Affective responses play a key role in exercise behavior, and transcranial direct current stimulation (tDCS), a non-invasive technique that applies low-intensity current to the scalp, may modulate these responses. However, evidence supporting its effectiveness remains equivocal. Objective: This study aimed to evaluate the effects of tDCS targeting the dorsolateral prefrontal cortex (DLPFC) on psychophysiological responses and brain oxygenation in healthy adults. Methods: Participants first completed a maximal incremental exercise test to assess exercise performance and aerobic fitness. In two subsequent sessions, participants received either active tDCS over the DLPFC or sham stimulation for 20 min, followed by a 20-min vigorous-intensity exercise session. Heart rate (HR) and brain oxygenation (measured via functional near-infrared spectroscopy, fNIRS) were continuously monitored during exercise. Affective valence, arousal, and rating of perceived exertion (RPE) were self-reported every 5 min. Data were analyzed using Generalized Estimating Equations and Generalized Mixed Models, with significance set at $p < 0.05$. Results: Brain oxygenation increased after exercise compared to baseline and post-tDCS ($p < 0.05$). However, tDCS did not significantly alter brain oxygenation at rest ($p > 0.3$) or during exercise ($p > 0.09$). No significant effect of tDCS was observed for the affective responses ($p > 0.08$), arousal ($p > 0.85$), or RPE (leg: $p > 0.90$; whole-body: $p > 0.28$). Conclusion: DLPFC-targeted tDCS does not modulate brain oxygenation or enhance psychophysiological responses during vigorous-intensity exercise in healthy individuals. Future studies should explore exercise preference and tolerance, and the effects of tDCS on clinical populations.

FRONTIERS IN PHYSIOLOGY 16, 1703766, 2025. DOI: 10.3389/fphys.2025.1703766. Acesso: <https://doi.org/10.3389/fphys.2025.1703766>

[P317-2025] “Electronic, optical, and mechanical properties of novel h-C10N3 and h-C9N4 carbon nitride monolayers from first principles”

Laranjeira, J. A. S.; Lima, K. A. L.*; Martins, N. F.; Aparicio-Huacarpuma, B. D.; Ribeiro Jr., L. A.; Sambrano, J. R.

Context We theoretically designed and systematically characterized two novel two-dimensional carbon nitride monolayers, h-C10N3 and h-C(9)N4, based on interconnected acepentalene motifs. Using density functional theory (DFT), we demonstrated their structural stability, confirmed by cohesive energies of - 6.89 eV/atom and - 6.92 eV/atom, respectively. Dynamical stability was validated by phonon calculations, revealing no significant imaginary frequencies,

while ab initio molecular dynamics simulations showed thermal robustness at 300 K. Both monolayers exhibit metallic behavior, dominated by carbon and nitrogen pz orbitals near the Fermi level. Optical analysis revealed low reflectance and strong absorption peak at 2.2 eV for h-C9N4 and broad absorption within 1.8-3.1 eV for h-C10N3, suggesting potential as visible-light absorbers. Mechanical characterization indicated high elastic stiffness (Young's modulus, 71-77 N/m), substantial shear resistance (23-25 N/m), and isotropic mechanical behavior (Poisson's ratio, 0.55). Our findings position these new carbon nitride monolayers as promising candidates for flexible electronic devices, photodetection, and optoelectronic applications. Methods First principles were performed using density functional theory (DFT) as implemented in VASP. The PBE functional with PAW pseudopotentials was employed, with a plane-wave cutoff of 520 eV. Thermal stability was assessed by ab initio molecular dynamics (AIMD) simulations at 300 K.

JOURNAL OF MOLECULAR MODELING 31[12], 328, 2025. DOI: 10.1007/s00894-025-06569-4. Acesso: <https://doi.org/10.1007/s00894-025-06569-4>

[P318-2025] "Elliptic anisotropy measurement of the f(980) hadron in proton-lead collisions and evidence for its quark-antiquark composition"

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

Despite the f(0)(980) hadron having been discovered half a century ago, the question about its quark content has not been settled: it might be an ordinary quark-antiquark ($q\bar{q}$) meson, a tetraquark ($qq\bar{q}\bar{q}$) exotic state, a kaon-antikaon ($K\bar{K}$) molecule, or a quark-antiquark-gluon ($q\bar{q}g$) hybrid. This paper reports strong evidence that the f(0)(980) state is an ordinary $q\bar{q}$ meson, inferred from the scaling of elliptic anisotropies (v_2) with the number of constituent quarks (n_q), as empirically established using conventional hadrons in relativistic heavy ion collisions. The f(0)(980) state is reconstructed via its dominant decay channel $f(0)(980) \rightarrow \pi^+\pi^-$, in proton-lead collisions recorded by the CMS experiment at the LHC, and its v_2 is measured as a function of transverse momentum (p_T). It is found that the $n_q = 2$ ($q\bar{q}$) hypothesis is favored over $n_q = 4$ ($qq\bar{q}\bar{q}$) or $K\bar{K}$ states by 7.7, 6.3, or 3.1 standard deviations in the $p_T < 10, 8, \text{ or } 6$ GeV/c ranges, respectively, and over $n_q = 3$ ($q\bar{q}g$) hybrid state by 3.5 standard deviations in the $p_T < 8$ GeV/c range. This result represents the first determination of the quark content of the f(0)(980) state, made possible by using a novel approach, and paves the way for similar studies of other exotic hadron candidates.

NATURE COMMUNICATIONS 16[1], 7990, 2025. DOI: 10.1038/s41467-025-56200-6. Acesso: <https://doi.org/10.1038/s41467-025-56200-6>

[P319-2025] "Engineered 3D-printed Bi4O5I2@hematite scaffolds for visible light photocatalytic degradation of cresols"

Rawat, A.; Oliveira, R. B. de*; Pal, T.; Lima, K. A. L.*; Fabris, G. S. L.*; Tromer, R. M.; Pereira Jr., M. L.; Singh, A.; Gupta, A. K.; Galvao, D. S.*; Tiwary, C. S.

Catalyst leaching hampers reusability in photocatalysis, posing secondary pollution risks. In the present study, Bi4O5I2 is decorated onto an engineered 3D-printed hematite scaffold (Bi4O5I2@3DH), integrating additive manufacturing with photocatalysis for efficient cresol degradation in diverse water matrices. The hematite grid, fabricated via direct ink writing, exhibited excellent rheological behavior ($\tau_y = 24$ Pa),

allowing precise shape retention, while Bi4O5I2 was immobilized via a simple dip-coating method. The Bi4O5I2@3DH composite achieved 99.78% degradation of 20 mg L⁻¹ p-cresol within 240 min and retained 84.28% efficiency after 10 reuse cycles with negligible leaching. Density functional theory (DFT+U) simulations confirmed S-scheme heterojunction formation, facilitating interfacial charge transfer (approximate to 0.9 e⁻) and enhanced photocatalytic activity. The engineered scaffold performed consistently across varied water matrices, with in vitro and in silico analyses revealing reduced toxicity of degradation products. The current work demonstrates a scalable strategy for coupling additive manufacturing with advanced photocatalysis using earth-abundant minerals for sustainable water treatment.

JOURNAL OF MATERIALS CHEMISTRY A, 2025. DOI: 10.1039/d5ta07867a Early Access Date: NOV 2025. Acesso: <https://doi.org/10.1039/D5TA07867A>

[P320-2025] "Eugenol as a synergistic adjuvant to conventional antibiotics against multidrug-resistant Klebsiella pneumoniae: An integrated in vitro and quantum-based in silico approach"

Barros, A. V.; Veras, B. O. de; Menezes, G. de L.; Bezerra, K. S.*; Galvao, D. S.*; et al.

The escalating antimicrobial resistance of *Klebsiella pneumoniae* poses a critical public health challenge, demanding innovative therapeutic strategies. This study investigated the antibacterial activity of eugenol (EOL) and its potential as a resistance-modulating agent when combined with conventional antibiotics—amoxicillin (AXL), azithromycin (AZT), cephalexin (CEF), and ciprofloxacin (CIP)—against clinical multidrug-resistant isolates. EOL exhibited intrinsic antibacterial activity with MIC values ranging from 1024 to 2048 μ g/mL. Checkerboard assays revealed synergistic interactions between EOL and AXL or AZT (FICI \leq 0.5), while combinations with CEF and CIP were indifferent. These synergistic effects were corroborated by growth inhibition curves, time-kill kinetics, and biofilm suppression assays, all of which demonstrated a marked reduction in bacterial viability and biofilm formation. Molecular docking and quantum mechanical calculations further elucidated the enhanced binding affinities and intermolecular interactions between AXL-EOL complexes and key resistance-related targets (KPC, LpxC, and particularly the quorum-sensing regulator SdiA), with interaction energies reaching up to -52.06 kcal/mol. Altogether, the findings underscore the potential of EOL as a potent adjuvant that augments the efficacy of conventional antibiotics, offering a promising pathway toward the development of targeted therapies against multidrug-resistant *K. pneumoniae*.

MICROBIAL PATHOGENESIS 210, 108126, 2025. DOI: 10.1016/j.micpath.2025.108126. Acesso: <https://doi.org/10.1016/j.micpath.2025.108126>

[P321-2025] "Evidence for a field-induced Lifshitz transition in the Weyl semimetal CeAlSi"

Piva, M. M.; Helm, T.; Souza, J. C.*; Pakuszewski, K. R.*; Adriano, C.*; Pagliuso, P. G.*; Nicklas, M.

The Weyl semimetal CeAlSi crystallises in the noncentrosymmetric tetragonal space group I41md and exhibits ferromagnetic order below 8 K, thereby breaking both spatial inversion and time-reversal symmetries. This unique combination of properties establishes CeAlSi as a model system for studying the interplay between non-trivial topological states and strong electron correlations. In this work, we report observations of Shubnikov-de Haas oscillations in the electrical resistivity under magnetic fields up to 68 T applied parallel to the [001] crystallographic axis. Our measurements reveal an abrupt change in the oscillation frequencies near 14 T,

which is indicative of a field-induced Lifshitz transition. Additionally, our results are consistent with the ferromagnetic order bringing the Weyl nodes closer to the Fermi level in CeAlSi. Furthermore, they suggest that the RKKY interaction plays an important role.

JOURNAL OF PHYSICS-CONDENSED MATTER 37[41], 415704, 2025. DOI: 10.1088/1361-648X/ae0be0. Acesso: <https://iopscience.iop.org/article/10.1088/1361-648X/ae0be0>

[P322-2025] “First measurement of symmetric cumulants of hexagonal flow harmonics in Pb-Pb collisions at $\sqrt{s_{NN}}=5.02$ TeV”

Acharya, S.; Agarwal, A.; Rinella, G. A.; Jahnke, C.*; Liveraro, G. S. S.*; Takahashi, J.*; et al.
ALICE Collaboration

Correlations between event-by-event fluctuations of anisotropic flow harmonics are measured in Pb-Pb collisions at a center-of-mass energy per nucleon pair of 5.02 TeV, as recorded by the ALICE detector at the LHC. This study presents correlations up to the hexagonal flow harmonic v_6 , which was measured for the first time. The magnitudes of these higher-order correlations are found to vary as a function of collision centrality and harmonic order. These measurements are compared to viscous hydrodynamic model calculations with EKRT initial conditions and to the iEBE-VISHNU model with TRENTo initial conditions. The observed discrepancies between the data and the model calculations vary depending on the harmonic combinations. Due to the sensitivity of model parameters estimated with Bayesian analyses to these higher-order observables, the results presented in this work provide new and independent constraints on the initial conditions and transport properties in theoretical models used to describe the system created in heavy-ion collisions.

PHYSICAL REVIEW C 112[2], 024905, 2025. DOI: 10.1103/4ltm-g1qg. Acesso: <https://doi.org/10.1103/4ltm-g1qg>

[P323-2025] “fNIRS reproducibility varies with data quality, analysis pipelines, and researcher experience”

Yücel, M. A.; Luke, R.; Mesquita, R. C.*; Martins, G. G.*; et al.

As data analysis pipelines grow more complex in brain imaging research, understanding how methodological choices affect results is essential for ensuring reproducibility and transparency. This is especially relevant for functional Near-Infrared Spectroscopy (fNIRS), a rapidly growing technique for assessing brain function in naturalistic settings and across the lifespan, yet one that still lacks standardized analysis approaches. In the fNIRS Reproducibility Study Hub (FRESH) initiative, we asked 38 research teams worldwide to independently analyze the same two fNIRS datasets. Despite using different pipelines, nearly 80% of teams agreed on group-level results, particularly when hypotheses were strongly supported by literature. Teams with higher self-reported analysis confidence, which correlated with years of fNIRS experience, showed greater agreement. At the individual level, agreement was lower but improved with better data quality. The main sources of variability were related to how poor-quality data were handled, how responses were modeled, and how statistical analyses were conducted. These findings suggest that while flexible analytical tools are valuable, clearer methodological and reporting standards could greatly enhance reproducibility. By identifying key drivers of variability, this study highlights current challenges and offers direction for improving transparency and reliability in fNIRS research.

COMMUNICATIONS BIOLOGY 8[1], 1149, 2025. DOI: 10.1038/s42003-025-08412-1. Acesso: <https://doi.org/10.1038/s42003-025-08412-1>

[P324-2025] “Gaussian generally covariant hydrodynamics”

Sampaio, G. M.*; Rabelo-Soares, G.*; Torrieri, G.*

We develop a version of fluctuating relativistic hydrodynamics in a way very different from the usual derivation: Instead of treating it as a coarse-grained deterministic theory expanded in gradients of equilibrium quantities, we treat it as a stochastic theory, characterized by partition functions in each cells, expanded in cumulants. We show that the Gaussian ansatz allows us, via the gravitational Ward identities acting as a constraint between the variance and the average, to maintain full general covariance, with hydrodynamic flow emerging as an approximate Killing vector. If the symmetry of ideal hydrodynamics, volume-preserving diffeomorphisms, is preserved, we show that linear response formulas are also generally covariant. We discuss our results and argue that in this approach, the applicability of the effective theory is parametrized around a very different quantity than the Knudsen number, offering hope of understanding the applicability of hydrodynamics to small systems.

PHYSICAL REVIEW D 112[5], 056002, 2025. DOI: 10.1103/67x1-knzz. Acesso: <https://doi.org/10.1103/67x1-knzz>

[P325-2025] “Graphene Heterostructure-Based Non-Volatile Memory Devices with Top Floating Gate Programming”

Rodrigues, G. L.*; Yoshida, A. B.*; Selmi, G. S.*; Jesus, N. T. K. B. de; Silva, I. R. F. E. e; Watanabe, K.; Taniguchi, T.; Oliveira, R. F. de; Lopez-Richard, V.; Cadore, A. R.

We present a graphene-based memory platform built on dual-gated field-effect transistors (GFETs). By integrating a lithographically defined metal patch directly atop the hexagonal boron nitride (hBN)-graphene channel, the device functions simultaneously as a top gate, floating gate (FG) reservoir, and active reset contact. This architecture forms an ultrathin van der Waals heterostructure with strong capacitive coupling to the back-gate, confirmed by a dynamic model, enabling a tunable and wide memory window that scales with back-gate voltage and is further enhanced by reducing hBN thickness or increasing FG area. Our devices demonstrate reversible, high-efficiency (>90%) charge programming, robust nonvolatile behavior across 10-300 K and a wide range of operation speeds, and endurance beyond 9800 cycles. Importantly, a grounded top electrode provides on-demand charge erasure, offering functionality that is absent in standard FG designs. These results position hBN/graphene-based GFETs as a compact, energy-efficient platform for next-generation 2D flash memory, with implications for multilevel memory schemes and cryogenic electronics.

ACS APPLIED ELECTRONIC MATERIALS 7[22], p. 10081-10089, 2025. DOI: 10.1021/acsaelm.5c01472. Acesso: <https://doi.org/10.1021/acsaelm.5c01472>

[P326-2025] “Impact Resistance of Complex 3D-Printed Schwarzites Structures”

Ambekar, R. S.; Oliveira, E. F.; Pugazhenth, P.; Singh, S.; Mahapatra, D. R.; Galvao, D. S.*; Tiwary, C. S.

Schwarzites are 3D carbon allotropes with negative Gaussian curvatures. Herein, the ballistic impact resistance and structures experimentally and energy-absorption capabilities of schwarzites from the gyroid and primitive families are investigated. Atomic and their corresponding 3D-printed structural models are investigated. In the schwarzite family, Omega 2 and Psi 2 have sustained the impact with minimal damage. The tested structures are further scanned using computer tomography to reveal and investigate their internal damage features. Molecular dynamics simulation results are in good agreement with the impact tests of the 3D-printed structures,

suggesting that the mechanical properties are determined mainly by the topological features and are scale-independent. The results point out that the performance of schwarzites structures is related to their local curvature, i.e., their flatness due to their ratio of hexagons to octagons. In general, the lower the ratio of hexagons to octagons, the stiffer the structure. Controlled mechanical response is possible by designing hierarchical schwarzite structures, making these structures good candidates for applications requiring lightweight materials with high resistance to ballistic impacts.

ADVANCED ENGINEERING MATERIALS, 2025. DOI: 10.1002/adem.202502191 Early Access Date: DEC 2025. Acesso: <https://doi.org/10.1002/adem.202502191>

[P327-2025] “Influence of temperature and pressure on preparing Ga nanowire arrays by press-based nanoinfiltration”

Mendonça, A. A.*; Tomiatti, L.*; Pirola, K. R.*; Béron, F.*

Nanoscale advanced materials are crucial for technological innovations. Among them, nanowires stand out due to their promising confinement effects and anisotropic properties derived from their elongated structure. However, this class of nanomaterials remains relatively underexploited, primarily due to fabrication challenges. In this work, we implement an alternative method for preparing nanowire arrays by pressing liquid metal into nanoporous alumina templates with cylindrical pores. Gallium was used as the liquid metal due to its melting point near room temperature. An investigation exploring the impact of temperature and pressure on the infiltration factor and length of nanowires was performed, revealing some counterintuitive behaviors. Higher filling factors and longer nanowires were obtained at lower infiltration temperatures, closer to the solidification point, with better performance observed at intermediate infiltration pressures rather than at higher pressures. Under optimal conditions, over 10 million parallel Ga nanowires per square millimeter were produced, with an average diameter of $151 + 36$ nm and a high aspect ratio of around 500.

NANOSCALE ADVANCES, 2025. DOI: 10.1039/d5na00640f. Early Access Date: NOV 2025. Acesso: <https://doi.org/10.1039/D5NA00640F>

[P328-2025] “Investigating the p - π^\pm and p - p - π^\pm dynamics with femtoscopy in pp collisions at $\sqrt{s}=13$ TeV”

Acharya, S.; Agarwal, A.; Rinella, G. A.; Guardiano, G. G.*; Liveraro, G. S. S.*; Takahashi, J.*; et al.
ALICE Collaboration

The interaction between pions and nucleons plays a crucial role in hadron physics. It represents a fundamental building block of the low-energy QCD dynamics and is subject to several resonance excitations. This work studies the p - π ($+/-$) dynamics using femtoscopic correlations in high-multiplicity pp collisions at $\sqrt{s} = 13$ TeV measured by ALICE at the LHC. As the final-state interaction between protons and pions is well constrained by scattering experiments and the study of pionic hydrogen, the results give access to information on the particle-emitting source in pp collisions using the femtoscopy methods. The scaling of the source size of primordial protons and pions against their pair transverse mass is extracted. The results are compared with the source sizes studied with p - p , p - K^+ , and π ($+/-$)- π ($+/-$) pairs by ALICE in the same collision system and are found to be in agreement for the different particle pairs. This reinforces recent findings by ALICE of a common emission source for all hadron-pairs in pp collisions at LHC energies. Furthermore, the p - p - π ($+/-$) systems are studied using three-particle femtoscopy in pp collisions at $\sqrt{s} = 13$ TeV.

The presence of three-body effects is analyzed utilizing the cumulant expansion method. In this formalism, the known two-body interactions are subtracted in order to isolate the three-body effects. For both, p - p - π ($+$) and p - p - π ($-$), a non-zero cumulant is found, indicating effects beyond pairwise interactions. These results give information on the coupling of the pion to multiple nucleons.

EUROPEAN PHYSICAL JOURNAL A 61[8], 194, 2025. DOI: 10.1140/epja/s10050-025-01615-4. Acesso: <https://doi.org/10.1140/epja/s10050-025-01615-4>

[P329-2025] “Investigation of the structural and tribological effects of silicon and nitrogen doping in hydrogenated amorphous carbon coatings applied to AISI M35 high-speed steel substrates”

Ba, E. C. T.; Almeida, L. S. de; Danelon, M. R.; Martins, P. S.; Rossino, L. S.; Siervo, A. de*; Pereira, L. A. de M.; Santos, S. C.

Hydrogenated Amorphous Carbon Coatings have been used in forming and machining tools, demonstrating solid lubrication capabilities, chemical inertness, wear resistance, and a reduction in the coefficient of friction. However, studies still report adhesion issues, which are often correlated with the residual stress state. Doping techniques have been used to mitigate this problem and, additionally, to improve the tribological performance of the coatings. In this study, nitrogen and silicon doping techniques were applied to hydrogenated amorphous carbon coatings deposited on AISI M35 high-speed steel. In the methodology, three types of coatings were deposited onto substrate samples and subsequently analyzed using structural, chemical, physical, and tribological characterization techniques. The results showed that nitrogen doping can increase sp^3 hybridizations more than silicon doping. The sp^3/sp^2 ratio appeared to be higher (0.56) with nitrogen doping compared to silicon (0.31). Nitrogen addition resulted in the hardest (ti 14 GPa) and stiffest (ti 130 GPa) coating, as well as the best adhesion to the substrate. Regarding silicon, the coating exhibited the greatest thickness (ti 5 μ m), the lowest hardness (ti 6 GPa) and stiffness (ti 46 GPa). Nevertheless, it showed the best performance in the micro-abrasive wear test: the worn volume represented only 4 % of the volume measured on the uncoated sample and also presented the lowest coefficient of friction (ti 0.1).

DIAMOND AND RELATED MATERIALS 159, 112902, 2025. DOI: 10.1016/j.diamond.2025.112902. Acesso: <https://doi.org/10.1016/j.diamond.2025.112902>

[P330-2025] “Light neutral-meson production in pp collisions at $\sqrt{s}=13$ TeV”

Acharya, S.; Agarwal, A.; Rinella, G. A.; Guardiano, G. G.*; Liveraro, G. S. S.*; Takahashi, J.*; et al.
ALICE Collaboration

The momentum-differential invariant cross sections of $\pi(0)$ and eta mesons are reported for pp collisions at $\sqrt{s} = 13$ TeV at midrapidity (vertical bar y vertical bar < 0.8). The measurement is performed in a broad transverse-momentum range of $0.2 < p(T) < 200$ GeV/c and $0.4 < p(T) < 60$ GeV/c for the $\pi(0)$ and eta, respectively, extending the $p(T)$ coverage of previous measurements. Transverse-mass-scaling violation of up to 60% at low transverse momentum has been observed, agreeing with measurements at lower collision energies. Transverse Bjorken x ($x(T)$) scaling of the $\pi(0)$ cross sections at LHC energies is fulfilled with a power-law exponent of $n = 5.01 \pm 0.05$, consistent with values obtained for charged pions at similar collision energies. The data are compared to predictions from next-to-leading order perturbative QCD calculations, where the $\pi(0)$ spectrum is best described using the CT18 parton distribution function and the NNFF1.0 or BDSS fragmentation function.

Expectations from PYTHIA8 and EPOS LHC overestimate the spectrum for the $\pi(0)$ and are not able to describe the shape and magnitude of the eta spectrum. The charged-particle multiplicity dependent $\pi(0)$ and eta $p(T)$ spectra show the expected change of the spectral shape, characterized by a flatter slope with increasing multiplicity. This is demonstrated across a broad transverse-momentum range and up to events with a charged-particle multiplicity exceeding five times the mean value in minimum bias collisions. The eta/ $\pi(0)$ ratio depends on the charged-particle multiplicity for $p(T) < 4$ GeV/c. PYTHIA8 and EPOS LHC qualitatively explain this behavior with an increasing contribution from the feed-down of heavier particles to the $\pi(0)$ spectrum.

JOURNAL OF HIGH ENERGY PHYSICS [8], 035, 2025. DOI: 10.1007/JHEP08(2025)035. Acesso: [https://doi.org/10.1007/JHEP08\(2025\)035](https://doi.org/10.1007/JHEP08(2025)035)

[P331-2025] “Linking Fundamentals and Devices: Evaluating Low Pt Ag Nanocatalysts in Three Electrode Systems and Operating Glycerol AEM Electrolyzers”

Lima, C. C.; Quispe, A. L. T.; Yukuhiro, V. Y.; Pires, C. T. G. V. M. T.; Silva, A. B. S.; Landers, R.*; Figueiredo, P. B. S. de; Lima, R. B. de; Arruda, M. A. Z.; Santos, K. T.; Linares, J. J.; Fernández, P. S.

Electro-oxidizing glycerol (GLOH) instead of water at the anode of an electrolyzer can lower the thermodynamic threshold potential by -1 V and simultaneously produce high-value-added products and green H_2 at the cathode. Herein, we report the use of Ag nanoparticles whose surfaces are enriched with low loadings of Pt (0.3-6.9 mol %) for the GLOH electro-oxidation reaction (GEOR). The optimized Pt(0.5%)Ag/C catalyst delivers $\sim 50\%$ of the geometric area normalized-activity of commercial Pt/C for GEOR in 0.5 M NaOH + 1 M GLOH, while using about 140 times less Pt. This remarkable performance originates from the synergy between Pt and Ag: Pt sites adsorb and initiate glycerol oxidation, while Ag sites provide oxygenated species that sustain the reaction and steer the product selectivity. Potential-dependent selectivity was observed: below 0.9 V vs RHE, glycerate and lactate dominate, whereas above 0.9 V, C-C scission yields glycolate and formate, with relatively low complete oxidation to carbonate. Device-level tests in an anion exchange membrane (AEM) electrolyzer corroborate half-cell trends. AgPt/C sustains current densities comparable to Pt/C but favors earlier formation of tartrate and higher glycerate production, confirming that the bimetallic interface modulates the reaction pathways. Both devices also show lactate, i.e., the product coming from a combination of an electrochemical and a chemical transformation. The combination of (i) drastically reduced noble-metal content, (ii) high activity at potentials well below the oxygen-evolution region, (iii) tunable co-production of C3 and C2 oxygenates, and (iv) cooperative Pt-Ag synergy, positions Pt-decorated Ag as a cost-effective anode platform for paired GLOH electro-reforming and green H_2 generation. Besides, we showed here that the catalysts are promising for other small organic molecules and that the results in three-electrode electrochemical cells, despite some limitations, help predict activity and selectivity trends for real devices.

ACS Electrochemistry 1[12], p. 2811-2822, 2025. DOI: 10.1021/acselectrochem.5c00366. Acesso: <https://pubs.acs.org/doi/10.1021/acselectrochem.5c00366>

[P332-2025] “Magnetic polaron formation in EuZn2P2”

Cook, M. S.; Peterson, E. A.; Kengle, C. S.; Kennedy, E. R.; Sheeran, J.; Girod, C.; Freitas, G. S.*; Greer, S. M.; Abbamonte, P.; Pagliuso, P. G.*; Thompson, J. D.; Thomas, S. M.; Rosa, P. F. S.

Colossal magnetoresistance (CMR) has been observed across many Eu $^{2+}$ -based materials; however, its origin is not completely understood. Here we investigate the antiferromagnetic insulator EuZn $2P_2$ through single crystal x-ray diffraction, transmission electron microscopy, electrical transport, magnetization, dilatometry, and electron spin resonance measurements complemented by density functional theory calculations. Our electrical resistivity data reveal a large negative magnetoresistance, $MR = [R(H)-R(0)]/R(0)$, that reaches $MR = -99.7\%$ at 9 T near the antiferromagnetic ordering temperature $T_N = 23$ K. Dilatometry measurements show an accompanying field-induced lattice strain. Additionally, Eu $^{2+}$ electron spin resonance reveals a strong ferromagnetic exchange interaction between Eu $^{2+}$ and conduction electrons. Our experimental results in EuZn $2P_2$ are consistent with a magnetic polaron scenario and suggest magnetic polaron formation as a prevailing explanation of CMR in Eu $^{2+}$ -based compounds.

PHYSICAL REVIEW MATERIALS 9[10], 104403, 2025. DOI: 10.1103/physrevmaterials.9.104403. Acesso: <https://doi.org/10.1103/physrevmaterials.9.104403>

[P333-2025] “Matter effects on flavor composition of astrophysical neutrinos”

Dev, P. S. B.; Jana, S.; Porto, Y.*

We show that high-energy astrophysical neutrinos produced in the cores of heavily obscured active galactic nuclei (AGNs) can undergo strong matter effects, thus significantly influencing their source flavor ratios. In particular, matter effects can completely modify the standard interpretation of the flavor ratio measurements in terms of the physical processes occurring in the sources (e.g., pp versus p gamma, full pion-decay chain versus muon-damped pion decay). We contrast our results with the existing flavor ratio measurements at IceCube, as well as with projections for next-generation neutrino telescopes like IceCube-Gen2. Signatures of these matter effects in neutrino flavor composition would not only bring more evidence for neutrino production in central AGN regions, but would also be a powerful probe of heavily Compton-thick AGNs, which escape conventional observation in x-rays and other electromagnetic wavelengths.

PHYSICAL REVIEW D 112[9], 093003, 2025. DOI: 10.1103/physrevd.112.093003. Acesso: <https://doi.org/10.1103/physrevd.112.093003>

[P334-2025] “Measurement of correlations among net-charge, net-proton, and net-kaon multiplicity distributions in Pb-Pb collisions at $\sqrt{s_{NN}}=5.02$ TeV”

Acharya, S.; Agarwal, A.; Rinella, G. A.; Jahnke, C.*; Liveraro, G. S. S.*; Takahashi, J.*; et al.
ALICE Collaboration

Correlations among conserved quantum numbers, such as the net-electric charge, the net-baryon, and the net-strangeness in heavy-ion collisions, are crucial for exploring the QCD phase diagram. In this paper, these correlations are investigated using net-proton number (as a proxy for the net-baryon), net-kaon number (for the net-strangeness), and net-charged particle number in Pb-Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV with the ALICE detector. The observed correlations deviate from the Poissonian baseline, with a more pronounced deviation at LHC energies than at RHIC. Theoretical calculations of the Thermal-FIST hadron resonance gas model, HIJING, and EPOS LHC event generators are compared with experimental results, where a significant impact of resonance decays is observed. Thermal-FIST calculations under the grand canonical and canonical ensembles highlight significant differences, underscoring the role of local charge conservation in explaining the data.

Recent lattice QCD studies have demonstrated that the magnetic field generated by spectator protons in heavy-ion collisions affects susceptibility ratios, in particular those related to the net-electric charge and the net-baryon numbers. The experimental findings are in qualitative agreement with the expectations of lattice QCD.

JOURNAL OF HIGH ENERGY PHYSICS [8], 210, 2025. DOI: 10.1007/JHEP08(2025)210. Acesso: [https://doi.org/10.1007/JHEP08\(2025\)210](https://doi.org/10.1007/JHEP08(2025)210)

[P335-2025] “Measurement of the W boson decay branching fraction ratio $B(W \rightarrow c\bar{q})/B(W \rightarrow q\bar{q})$ in proton-proton collisions at $\sqrt{s}=13\text{TeV}$ ”

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

The most precise measurement to date of the W boson hadronic decay branching fraction ratio $R_c(W) = B(W \rightarrow c\bar{q})/B(W \rightarrow q\bar{q})$ is presented. The measurement is based on a sample of proton-proton collision data from the CERN LHC collected by the CMS experiment at a center-of-mass energy of 13TeV in 2016-2018 with an integrated luminosity of 138 fb⁻¹. The large cross section of top quark-antiquark production at the LHC offers a sizable high-purity sample of W bosons suitable for this measurement. Events with one charged lepton (electron or muon) and at least four jets, two tagged as bottom quark jets, are analyzed. Charm jets are tagged using the presence of a muon inside the jet. The result, $R_c(W) = 0.489 \pm 0.020$, is consistent with the standard model prediction and is twice as precise as the current world-average value.

PHYSICS LETTERS B 868, 139754, 2025. DOI: 10.1016/j.physletb.2025.139754. Acesso: <https://doi.org/10.1016/j.physletb.2025.139754>

[P336-2025] “Measurements of differential two-particle number and transverse momentum correlation functions in pp collisions at $\sqrt{s}=13\text{TeV}$ ”

Acharya, S.; Agarwal, A.; Rinella, G. A.; Guardiano, G. G.*; Liveraro, G. S. S.*; Takahashi, J.*; et al.
ALICE Collaboration

Differential two-particle normalized cumulants (R-2) and transverse momentum correlations (P-2) are measured as a function of the relative pseudorapidity and azimuthal angle difference ($\Delta\eta$, $\Delta\phi$) of charged particle pairs in minimum bias pp collisions at $\sqrt{s} = 13\text{TeV}$. The measurements use charged hadrons in the pseudorapidity region of $|\eta| < 0.8$ and the transverse momentum range $0.2 < p_T < 2.0\text{GeV}/c$ in order to focus on soft multiparticle interactions and to complement prior measurements of these correlation functions in p-Pb and Pb-Pb collisions. The correlation functions are reported for both unlike-sign and like-sign pairs and their charge-independent and charge-dependent combinations. Both the R-2 and P-2 measured in pp collisions exhibit features qualitatively similar to those observed in p-Pb and Pb-Pb collisions. The $\Delta\eta$ and $\Delta\phi$ root mean square widths of the near-side peak of the correlation functions are evaluated and compared with those observed in p-Pb and Pb-Pb collisions and show smooth evolution with the multiplicity of charged particles produced in the collision. The comparison of the measured correlation functions with predictions from PYTHIA8 shows that this model qualitatively captures their basic structure and characteristics but feature important differences. In addition, the R-2(CD) is used to determine the charge balance function of hadrons produced within the detector acceptance of the measurements. The integral of the balance function is found to be compatible with those reported by a previous measurement in Pb-Pb collisions.

EUROPEAN PHYSICAL JOURNAL C 85[8], 866, 2025. DOI: 10.1140/epjc/s10052-025-14531-0. Acesso: <https://doi.org/10.1140/epjc/s10052-025-14531-0>

[P337-2025] “Medium-induced modification of groomed and ungroomed jet mass and angularities in Pb-Pb collisions at $\sqrt{s_{NN}}=5.02\text{TeV}$ ”

Acharya, S.; Agarwal, A.; Rinella, G. A.; Guardiano, G. G.*; Liveraro, G. S. S.*; Takahashi, J.*; et al.
ALICE Collaboration

The ALICE Collaboration presents a new suite of jet substructure measurements in Pb-Pb and pp collisions at a center-of-mass energy per nucleon pair $\sqrt{s_{NN}} = 5.02\text{TeV}$. These measurements provide access to the internal structure of jets via the momentum and angle of their constituents, probing how the quark-gluon plasma modifies jets, an effect known as jet quenching. Jet grooming additionally removes soft wide-angle radiation to enhance perturbative accuracy and reduce experimental uncertainties. We report the groomed and ungroomed jet mass $m(\text{jet})$ and jet angularities $\lambda(\kappa)(\alpha)$ using $\kappa = 1$ and $\alpha > 0$. Charged-particle jets are reconstructed at midrapidity using the anti-k(T) algorithm with resolution parameter $R = 0.2$. A narrowing of the jet mass and angularity distributions in Pb-Pb collisions with respect to pp is observed and is enhanced for groomed results, confirming modification of the jet core. By using consistent jet definitions and kinematic cuts between the mass and angularities for the first time, previous inconsistencies in the interpretation of quenching measurements are resolved, rectifying a hurdle for understanding how jet quenching arises from first principles and highlighting the importance of a well-controlled baseline. These results are compared with a variety of theoretical models of jet quenching, providing constraints on jet energy-loss mechanisms in the quark-gluon plasma.

PHYSICS LETTERS B 864, 139409, 2025. DOI: 10.1016/j.physletb.2025.139409. Acesso: <https://doi.org/10.1016/j.physletb.2025.139409>

[P338-2025] “Metal-decorated HOP-graphene as a promising media for high-capacity reversible hydrogen storage: Insights from DFT and AIMD simulations”

Martins, N. F.; Laranjeira, J. A. S.; Lima, K. A. L.*; Chen, X. H.; Ribeiro Jr., L. A.; Sambrano, J. R.

Two-dimensional (2D) materials have been extensively investigated for applications in gas sensing, catalysis, and energy storage, owing to their exceptional surface area and high structural tunability. In the context of addressing global warming and transitioning to cleaner energy alternatives, hydrogen-based energy systems have emerged as promising solutions. However, efficient hydrogen storage and release require the development of suitable substrate materials. In this study, we perform a comprehensive density functional theory (DFT) investigation of Li- and Na-decorated HOP-graphene, a 2D carbon allotrope characterized by its unique 5-6-8 ring configuration, as a candidate for hydrogen (H₂) storage. Our calculations reveal a remarkable hydrogen uptake capacity of 10.74 wt% and 8.85 wt% for Li and Na decoration, respectively, with both systems capable of accommodating up to 32 H₂ molecules. Moreover, the predicted desorption temperatures are close to room temperature, attributed to the presence of Kubas-type interactions. Ab initio molecular dynamics (AIMD) simulations further support this behavior, demonstrating substantial hydrogen release at 300 K without any structural degradation of the decorated substrate. These results position metal-decorated HOP-graphene as a highly promising and efficient material for next-generation hydrogen storage applications.

DIAMOND AND RELATED MATERIALS 160, 112980, 2025. DOI: 10.1016/j.diamond.2025.112980. Acesso: <https://doi.org/10.1016/j.diamond.2025.112980>

[P339-2025] “Multifunctional sensing of cobalt ions and methylcobalamin using doped Carbon Quantum Dots”

Oliveira, C. M. P.; Lima, F. E. H.; Lopes, G. S.; Matos, W. O.; Antunes, R. A.; Neto, M. L. A.*; Moura, T. A.; Paschoal, A. R.; Cesar, C. L.*; Carvalho, H. F.*; Freire, R. M.; Santos-Oliveira, R.; Fechine, P. B. A.; Carneiro, S. V.

In this work, a new fluorescent probe highly sensitive to Cobalt ions and Methylcobalamin (MC) was developed. For this purpose, sulfur- and nitrogen-doped carbon quantum dots (CQDs) with a Quantum Yield (QY) of 8 % were employed in a novel platform capable of discriminating different analytes in solution and detecting MC and Co²⁺ at concentrations as low as 1.36 ppm and 50.6 ppm, respectively. The MC, the active form of vitamin B12, is essential for DNA synthesis and neurological health. Its deficiency can lead to neuropathies and severe neurological disorders. It contains cobalt in its structure, a trace element recognized as vital for maintaining nervous system functions and erythropoiesis. Consequently, cobalt is also utilized by athletes to enhance performance during anaerobic exercise. The precise quantification of cobalt concentrations in the human body is crucial for the diagnosis of various pathologies and for the optimization of therapeutic interventions. The N,S-CDs were synthesized through a bottom-up approach, utilizing a hydrothermal method with citric acid, mercaptosuccinic acid (MSA), and ethylenediamine as precursor molecules. The efficient quenching of N,S-CDs fluorescence by Co²⁺ and MC was employed for the detection of these analytes, achieving a limit of detection (LOD) of 50.6 ppm for Co²⁺ and 1.36 ppm for MC, with recovery assays of 100.71 % and 99.33 % for Co²⁺ and MC, respectively. Furthermore, Co²⁺ and MC ions were identified in real water samples, in the presence of various interfering ions present in the solution, from Linear Discriminant Analysis (LDA), with 100 % of accuracy.

MICROCHEMICAL JOURNAL 217, 114930, 2025. DOI: 10.1016/j.microc.2025.114930. Acesso: <https://doi.org/10.1016/j.microc.2025.114930>

[P340-2025] “Multiplicity-dependent inclusive J/ψ production at forward rapidity in pp collisions at $\sqrt{s}=13$ TeV”

Acharya, S.; Agarwal, A.; Rinella, G. A.; Jahnke, C.*; Liveraro, G. S. S.*; Takahashi, J.*; et al.
ALICE Collaboration

This paper presents a study of the inclusive forward J/ψ yield as a function of forward charged-particle multiplicity in pp collisions at root s = 13 TeV using data collected by the ALICE experiment at the CERN LHC. The results are presented in terms of relative J/ψ yields and relative charged-particle multiplicities with respect to these quantities obtained in inelastic collisions having at least one charged particle in the pseudorapidity range $|\eta| < 1$. The J/ψ mesons are reconstructed via their decay into mu(+)mu(-) pairs in the forward rapidity region ($2.5 < y < 4$). The relative multiplicity is estimated in the forward pseudorapidity range which overlaps with the J/ψ rapidity region. The results show a steeper-than-linear increase of the J/ψ yields versus the multiplicity. They are compared with previous measurements and theoretical model calculations.

JOURNAL OF HIGH ENERGY PHYSICS [7], 238, 2025. DOI: 10.1007/JHEP07(2025)238. Acesso: [https://doi.org/10.1007/JHEP07\(2025\)238](https://doi.org/10.1007/JHEP07(2025)238)

[P341-2025] “Neural network based nodal structure optimization for interacting fermionic systems”

Freitas, W.*; Abreu, B.; Vitiello, S. A.*

Simulating strongly correlated fermionic systems remains a fundamental challenge in quantum physics, largely due to the sign problem in quantum Monte Carlo (QMC) methods. We present a neural network-based variational Monte Carlo (NN-VMC) approach, leveraging a flexible neural network ansatz to represent the many-body wavefunction. Focusing on quantum dots with up to 30 electrons, we demonstrate that NN-VMC significantly reduces variational bias and achieves ground-state energies surpassing those of fixed-node diffusion Monte Carlo (DMC). A key feature is that the neural network adaptively learns and optimizes nodal structures during energy minimization. We provide qualitative insights into the nodal structure of fermionic wavefunctions by comparing the nodal structures generated by NN-VMC with those obtained from traditional trial functions. Additionally, we reveal spin-resolved radial distributions and electron density profiles, highlighting the versatility and accuracy of NN-VMC. This work underscores the potential of machine learning to advance quantum simulations and deepen our understanding of strongly correlated systems.

PHYSICAL REVIEW B 112[16], 165109, 2025. DOI: 10.1103/x6cj-b6lj. Acesso: <https://doi.org/10.1103/x6cj-b6lj>

[P342-2025] “Non-local X-ray intermolecular radiative decay probes solvation shell of ions in water”

Söderström, J.; Cornetta, L. M.; Ekholm, V.; Carravetta, V.; Brito, A. N. de*; et al.

Aqueous solutions are crucial in chemistry, biology, environmental science, and technology. The chemistry of solutes is influenced by the surrounding solvation shell of water molecules, which have different chemical properties than bulk water due to their different electronic and geometric structure. It is experimentally challenging to selectively investigate this property-determining electronic and geometric structure. Here, we report experimental results on the non-local X-ray emission process Intermolecular Radiative Decay, for the prototypical ions Na⁺ and Mg²⁺ in water. We show that, in Intermolecular Radiative Decay, an electron from the solvation shell fills a core hole in the solute, and the released energy is emitted as an X-ray photon. We interpret the underlying mechanism using theoretical calculations, and show how Intermolecular Radiative Decay will allow us to meet the challenge of selectively probing the solvation shell from within.

NATURE COMMUNICATIONS 16[1], 10046, 2025. DOI: 10.1038/s41467-025-65581-7. Acesso: <https://doi.org/10.1038/s41467-025-65581-7>

[P343-2025] “Observation of WZγ production and constraints on new physics scenarios in proton-proton collisions at $\sqrt{s}=13$ TeV

Chekhovsky, V.; Hayrapetyan, A.; Chinellato, J. A.*; et al.
CMS Collaboration

A measurement of the WZ gamma triboson production cross section is presented. The analysis is based on a data sample of proton-proton collisions at a center-of-mass energy of root s = 13 TeV recorded with the CMS detector at the LHC, corresponding to an integrated luminosity of 138 fb⁻¹. The analysis focuses on the final state with three charged leptons, l(+/-)nu l(+)(-), where l = e or mu, accompanied by an additional photon. The observed (expected) significance of the WZ gamma signal is 5.4 (3.8) standard deviations.

The cross section is measured in a fiducial region, where events with an l originating from a tau lepton decay are excluded, to be 5.48 ± 1.11 fb, which is compatible with the prediction of 3.69 ± 0.24 fb at next-to-leading order in quantum chromodynamics. Exclusion limits are set on anomalous quartic gauge couplings and on the production cross sections of massive axionlike particles.

PHYSICAL REVIEW D 112[1], 012009, 2025. DOI: 10.1103/cm24-665b. Acesso: <https://doi.org/10.1103/cm24-665b>

[P344-2025] “Optical and Magnetic Response by Design in GaAs Quantum Dots”

Schimpf, C.; Garcia Jr., A. J.; Koong, Z. X.; Silva, S. F. C. da*; Ritzmann, J.*; Babin, H. G.*; Wieck, A. D. *; et al.

Quantum networking technologies use spin qubits and their interface to single photons as core components of a network node. This necessitates the ability to co-design the magnetic- and optical-dipole response of a quantum system—a capability that has been notably absent in solid-state platforms where spin-orbit coupling and the crystalline environment lead to inhomogeneity of electronic g -factors and optically active states. Here, we demonstrate the ability to design both the optical and magnetic response of a solid-state quantum emitter a priori. We show that GaAs quantum dots (QDs), obtained via local droplet etching epitaxy and already known as exceptionally coherent and efficient quantum light sources, also exhibit spin and optical properties that follow directly from assuming the highest possible system symmetry. Our measurements of electron and hole g -tensors—using a new sign-sensitive measurement protocol based on the hyperfine interaction—and of transition dipole moment orientations for charged excitons agree with our predictions from a multiband $k \cdot p$ simulation constrained only by a single atomic-force-microscopy reconstruction of QD morphology. This agreement is verified across multiple wavelength-specific growth runs at different facilities within the range of 730 to 790 nm for the exciton emission. Remarkably, our measurements and simulations track the in-plane electron g -factors through a zero-crossing from -0.1 to 0.3 and linear optical dipole moment orientations fully determined by an external magnetic field. The robustness and generality of these results establish a fundamentally new paradigm for solid-state spin-photon interfaces: one in which the properties of a spin qubit and its tunable optical interface can be designed-prior to growth-for a target magnetic and photonic environment, with direct applications to scalable and high-fidelity spin-photon entanglement.

PRX QUANTUM 6[4], 040309, 2025. DOI: 10.1103/98cp-1k42. Acesso: <https://doi.org/10.1103/98cp-1k42>

[P345-2025] “Optoelectronic and Excitonic Study of XI₂ (X = Si, Ge, Sn, and Pb) Monolayers Envisaging Potential Technological Applications”

Aparicio-Huacarpuma, B. D.; Laranjeira, J. A. dos S.; Lima, K. A. L.*; Moujaes, E. A.; Silva, A. M. A.; Sambrano, J. R.; Dias, A. C.; Ribeiro Jr., L. A.

This study investigates the structural stability and electronic, mechanical, excitonic, and optical properties of 2D-XI₂ (X = Si, Ge, Sn, Pb) monolayers using both first-principles and semiempirical calculations. Our findings reveal that this group has semiconductor characteristics with band gaps from 2.35 to 3.28 eV at the HSE06 level. The excitonic effects are significant with exciton binding energies between 372 and 422 meV. They present a maximum solar harvesting efficiency, at the Shockley-Queisser limit, considering an electron-hole coupling of 16.37%. These findings indicate that these structures are promising for future optoelectronic applications, showing excellent visible and ultraviolet response and enhancing the photovoltaic cell performance.

ACS OMEGA, 2025. DOI: 10.1021/acsomega.5c08479 Early Access Date: NOV 2025. Acesso: <https://doi.org/10.1021/acsomega.5c08479>

[P346-2025] “Performance of a Modular Ton-Scale Pixel-Readout Liquid Argon Time Projection Chamber”

Abud, A. A.; Abi, B.; Acciarri, R.; Adriano, C.*; Bazetto, M. C. Q.*; Borges Merlo, R.*; Aguiar, R. de*; Almeida, P. de*; Holanda, P. C. de*; Gelli, B.*; Gratieri, D. R.*; Guzzo, M. M.*; Kemp, E.*; Machado, A. A.*; Marques, F. das C.*; Peres, O. L. G.*; Pimentel, V. L.*; Segreto, E.*; et al
DUNE Collaboration

The Module-0 Demonstrator is a single-phase 600 kg liquid argon time projection chamber operated as a prototype for the DUNE liquid argon near detector. Based on the ArgonCube design concept, Module-0 features a novel 80k-channel pixelated charge readout and advanced high-coverage photon detection system. In this paper, we present an analysis of an eight-day data set consisting of 25 million cosmic ray events collected in the spring of 2021. We use this sample to demonstrate the imaging performance of the charge and light readout systems as well as the signal correlations between the two. We also report argon purity and detector uniformity measurements and provide comparisons to detector simulations.

INSTRUMENTS 8[3], 41, 2025. DOI: 10.3390/instruments8030041. Acesso: <https://doi.org/10.3390/instruments8030041>

[P347-2025] “Physics-informed generative adversarial networks applied to dichroic filters’ properties regression”

Rodrigues, M. J. de O.; Bazetto, M. C. Q.*; Machado, A. A. B.*; Dias, M. R. S.; Valdivieso, G. do A.; Bezerra, A. T.

Optical dichroic filters are key components of light detectors, and simulation is a desirable tool in detectors’ research and development (R&D). Simulations must address the nuances of light-matter interactions to provide a realistic representation of the detector’s performance. Accessing this information requires experimental data and precise measurements of the optical response under various conditions. While first-principles simulations are feasible, they are computationally costly and struggle to capture imperfections of real devices. To address this, we present the use of machine learning employing a conditional physics-informed generative adversarial network (CPIGAN) to simulate the optical transmittance of dichroic filters. Training on measured and simulated data enables the prediction of the filter’s behavior, capturing deviations between experiment and simulation, thereby shifting the bulk of the computational effort to training. Through training on datasets with varying numbers of experimental curves, we demonstrated that employing an optimized CPIGAN architecture with physics-informed loss terms enables the generation of realistic synthetic transmittance curves, even in scenarios with limited experimental data. We demonstrated good training results through a trade-off between properly selecting the experimental representative samples and robust hyperparameter optimization. We foresee that the plasticity of the CPIGAN model will be essential for handling diverse filter designs, enabling reliable, effective, and precise ML-assisted simulations.

PHYSICA SCRIPTA 100[11], 116012, 2025. DOI: 10.1088/1402-4896/ae1f50. Acesso: <https://iopscience.iop.org/article/10.1088/1402-4896/ae1f50>

[P348-2025] “Quantum teleportation with dissimilar quantum dots over a hybrid quantum network”

Laneve, A.; Ronco, G.; Beccaceci, M.; Covre da Silva, S. F.*; et al.

Photonic quantum information processing in metropolitan quantum networks lays the foundation for cloud quantum computing, secure communication, and the realization of a global quantum internet. This paradigm shift requires on-demand and high-rate generation of flying qubits and their quantum state teleportation over long distances. Despite the last decade has witnessed an impressive progress in the performances of deterministic photon sources, the exploitation of distinct quantum emitters to implement a quantum relay among distant parties has remained elusive. Here, we overcome this challenge by using dissimilar quantum dots whose electronic and optical properties are engineered by light-matter interaction, multi-axial strain and magnetic fields so as to make them suitable for the teleportation of polarization qubits. This is demonstrated in a quantum network harnessing both fiber connections and a 270 m free-space optical link connecting two buildings of the Sapienza University campus in Rome. The protocol exploits GPS-assisted synchronization, ultra-fast single photon detectors as well as stabilization systems that compensate for atmospheric turbulence. The achieved teleportation state fidelity reaches up to $82 \pm 1\%$, above the classical limit by more than 10 standard deviations. Our field demonstration of all-photonic quantum teleportation opens a new route to implement solid-state based quantum relays and builds the foundation for practical quantum networks.

NATURE COMMUNICATIONS 16[1], 10028, 2025. DOI: 10.1038/s41467-025-65911-9. Acesso: <https://doi.org/10.1038/s41467-025-65911-9>

[P349-2025] “Radio frequency-induced catalysis using multi-component two-dimensional quasicrystals for effective sulfamethoxazole removal from water”

Manzoor, Z.; Karthik, R.; Ferreira, M. A.; Galvao, D. S.*; Mukhopadhyay, N. K.; Yadav, T P.; Dadhwal, P.; Saka, P. C.; Woellner, C. F.; Chowdhury, S.; Tiwary, C. S.

This study presents a novel strategy for removing pharmaceutical pollutants from aqueous media using radio frequency (RF)-assisted catalysis with two-dimensional (2D) AlFeCoNiCu quasicrystals (QCs). The QCs were synthesized via liquid-phase exfoliation of the corresponding bulk alloy and exposed to 35 MHz RF irradiation to assess their catalytic performance. Under these conditions, the 2D QCs achieved 55 % removal of sulfamethoxazole (SMX) within 10 min, nearly double the efficiency of control systems. This performance is attributed to enhanced electrical conductivity, improved RF penetration, and localized surface heating, as confirmed by thermal imaging. In situ transmission electron microscopy and combined density functional theory/molecular dynamics simulations revealed progressive SMX degradation, facilitated by charge transfer from Ni-rich active sites, confirming the catalytic role of the QCs. These findings demonstrate that RF-activated 2D QCs provide a magnetically recoverable, energy-efficient, and scalable platform for pharmaceutical pollutant removal, offering a sustainable solution for next-generation water treatment technologies.

APPLIED CATALYSIS B-ENVIRONMENT AND ENERGY 383, 126062, 2025. DOI: 10.1016/j.apcatb.2025.126062. Acesso: <https://doi.org/10.1016/j.apcatb.2025.126062>

[P350-2025] “Reporting on pTP sublimation during evaporation deposition”

Gomes, G.*; Gelli, B.*; Palaveri, V. C.*; Sola, R.*; Marques, F. C.*; Kemp, E.*

Noble liquid detectors rely on wavelength shifter materials, such as p-terphenyl (pTP) and tetraphenyl-butadiene (TPB),

which are widely used in neutrino and dark matter experiments. Given their importance, a thorough understanding and characterization of these compounds are essential for optimizing experimental techniques and enhancing detector performance. In this study, we report a novel phenomenon in which commonly used wavelength shifters undergo spontaneous sublimation under high-vacuum conditions. We quantify the sublimation rates of pTP and TPB as a function of pressure and temperature, and evaluate their impact on material growth and physical properties. Furthermore, we investigate how variations in film thickness and growth rate influence the sublimation process. These findings provide critical insights into the handling and preparation of wavelength shifters during the fabrication of light detectors for these experiments, ensuring their stability and reliability in low-background photodetection systems.

JOURNAL OF INSTRUMENTATION 20[10], C10016, 2025. DOI: 10.1088/1748-0221/20/10/C10016. Acesso: <https://iopscience.iop.org/article/10.1088/1748-0221/20/10/C10016>

[P351-2025 “Revisiting the Jaynes-Cummings Model with Time-dependent Coupling”

Tsutsui, T. T.; Cius, D.; Vidiella-Barranco, A.*; Castro, A. S. M. De; Andrade, F. M.

The Jaynes-Cummings (JC) model stands as a fully quantized, fundamental framework for exploring light-matter interactions, a timely reflection on a century of quantum theory. The time-dependent Jaynes-Cummings (TDJC) model introduces temporal variations in certain parameters, which often require the use of numerical methods. However, under the resonance condition, exact solutions can be obtained, offering insight into a variety of physical scenarios. In this work, we study the resonant TDJC model considering different modulations of the atom-field coupling. The model is presented and an analytical solution derived in a didactic way, allowing us to examine how time-dependent couplings affect atomic population inversion and atom-field entanglement. We also consider an atom traversing a partially cooled cavity, which induces periodicity and reveals the combined effects of atomic motion and thermal fluctuations. The Bloch vector is used to analyze the dynamics of the system, including the atomic state purity, and reveals phenomena such as atomic dipole alignment with the field due to the oscillating coupling, as well as atomic population trapping, which arises by increasing the initial mean thermal photon number.

BRAZILIAN JOURNAL OF PHYSICS 56[1], 21, 2025. DOI: 10.1007/s13538-025-01949-w. Acesso: <https://doi.org/10.1007/s13538-025-01949-w>

[P352-2025] “Search for bosons of an extended Higgs sector in b quark final states in proton-proton collisions at $\sqrt{s}=13$ TeV”

Chekhovsky, V.; Hayrapetyan, A.; Makarenko, V.; Chinellato, J. A.*; et al.
CMS Collaboration

A search for beyond-the-standard-model neutral Higgs bosons decaying to a pair of bottom quarks, and produced in association with at least one additional bottom quark, is performed with the CMS detector. The data were recorded in proton-proton collisions at a centre-of-mass energy of 13 TeV at the CERN LHC and correspond to an integrated luminosity of 36.7-126.9 fb⁻¹, depending on the probed mass range. No signal above the standard model background expectation is observed. Upper limits on the production cross section times branching fraction are set for Higgs bosons in the mass range of 125-1800 GeV. The results are interpreted in benchmark scenarios of the minimal supersymmetric standard model, as well as suitable classes of two-Higgs-doublet models.

JOURNAL OF HIGH ENERGY PHYSICS [6], 144, 2025. DOI: 10.1007/JHEP06(2025)144. Acesso: [https://doi.org/10.1007/JHEP06\(2025\)144](https://doi.org/10.1007/JHEP06(2025)144)

[P353-2025] “Search for excited tau leptons in the $\tau\tau$ final state in proton-proton collisions $\sqrt{s}=13$ TeV”

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

Results are presented for a test of the compositeness of the heaviest charged lepton, tau, using data collected by the CMS experiment in proton-proton collisions at a center-of-mass energy of 13 TeV at the CERN LHC. The data were collected in 2016-2018 and correspond to an integrated luminosity of 138 fb⁻¹. This analysis searches for tau lepton pair production in which one of the tau leptons is produced in an excited state and decays to a ground state tau lepton and a photon. The event selection consists of two isolated tau lepton decay candidates and a high-energy photon. The mass of the excited tau lepton is reconstructed using the missing transverse momentum in the event, assuming the momentum of the neutrinos from each tau lepton decay are aligned with the visible decay products. No excess of events above the standard model background prediction is observed. This null result is used to set lower bounds on the excited tau lepton mass. For a compositeness scale Λ equal to the excited tau lepton mass, excited tau leptons with masses below 4700 GeV are excluded at 95% confidence level; for $\Lambda = 10$ TeV this exclusion is set at 2800 GeV. This is the first experimental result covering this production and decay process in the excited tau mass range above 175 GeV.

JOURNAL OF HIGH ENERGY PHYSICS [6], 006, 2025. DOI: 10.1007/JHEP06(2025)006. Acesso: [https://doi.org/10.1007/JHEP06\(2025\)006](https://doi.org/10.1007/JHEP06(2025)006)

[P354-2025] “Search for medium effects using jet axis decorrelation in inclusive jets from PbPb collisions at $\sqrt{s_{NN}}=5.02$ TeV”

Chekhovsky, V.; Hayrapetyan, A.; Makarenko, V.; Chinellato, J. A.*; et al.
CMS Collaboration

The jet axis decorrelation in inclusive jets is studied using lead-lead (PbPb) collisions at a center-of-mass energy per nucleon pair of 5.02 TeV. The jet axis decorrelation is defined as the angular difference between two definitions of the jet axis. It is obtained by applying two recombination schemes on all the constituents of a given jet reconstructed by the anti-k(T) sequential algorithm with a distance parameter of $R = 0.4$. The data set, corresponding to an integrated luminosity of 0.66 nb⁻¹, was collected in 2018 with the CMS detector at the CERN LHC. The jet axis decorrelations are examined across collision centrality selections and intervals of jet transverse momentum. A centrality dependent evolution of the measured distributions is observed, with a progressive narrowing seen in more central events. This narrowing could result from medium-induced modification of the internal jet structure or reflect color charge effects in energy loss. This new measurement probes jet substructure in previously unexplored kinematic domains and show great promise for providing new insights on the color charge dependence of energy loss to jet-quenching models.

JOURNAL OF HIGH ENERGY PHYSICS [6], 120, 2025. DOI: 10.1007/JHEP06(2025)120. Acesso: [https://doi.org/10.1007/JHEP06\(2025\)120](https://doi.org/10.1007/JHEP06(2025)120)

[P355-2025] “Search for Nuclear Modifications of B+ Meson Production in p-Pb Collisions at $\sqrt{s_{NN}}=8.16$ TeV”

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

Nuclear medium effects on B+ meson production are studied using the binary-collision scaled cross section ratio between events of different charged-particle multiplicities from proton-lead collisions. Data, collected by the CMS experiment in 2016 at a nucleon-nucleon center-of-mass energy of $\sqrt{s_{NN}} = 8.16$ TeV, corresponding to an integrated luminosity of 175 nb⁻¹, were used. The scaling factors in the ratio are determined using a novel approach based on the $Z \rightarrow \mu(-)\mu(+)$ cross sections measured in the same events. The scaled ratio for B+ is consistent with unity for all event multiplicities, putting stringent constraints on nuclear modification for heavy flavor.

PHYSICAL REVIEW LETTERS 134[11], 111903, 2025. DOI: 10.1103/PhysRevLett.134.111903. Acesso: <https://doi.org/10.1103/PhysRevLett.134.111903>

[P356-2025] “Search for Quasiparticle Scattering in the Quark-Gluon Plasma with Jet Splittings in pp and Pb-Pb Collisions at $\sqrt{s_{NN}}=5.02$ TeV”

Acharya, S.; Agarwal, A.; Rinella, G. A.; Guardiano, G. G.*; Livanaro, G. S. S.*; Takahashi, J.*; et al.
ALICE Collaboration

The ALICE Collaboration reports measurements of the large relative transverse momentum ($k(T)$) component of jet substructure in pp and Pb-Pb collisions at center-of-mass energy per nucleon pair $\sqrt{s_{NN}} = 5.02$ TeV. Enhancement in the yield of such large- $k(T)$ emissions in head-on Pb-Pb collisions is predicted to arise from partonic scattering with quasiparticles of the quark-gluon plasma. The analysis utilizes charged-particle jets reconstructed by the anti-kT algorithm with resolution parameter $R = 0.2$ in the transverse-momentum interval $60 < p(T, \text{ch, jet}) < 80$ GeV/c. The soft drop and dynamical grooming algorithms are used to identify high transverse momentum splittings in the jet shower. Comparison of measurements in Pb-Pb and pp collisions shows medium-induced narrowing, corresponding to yield suppression of high- $k(T)$ splittings, in contrast to the expectation of yield enhancement due to quasiparticle scattering. The measurements are compared to theoretical model calculations incorporating jet modification due to jet-medium interactions (“jet quenching”), both with and without quasiparticle scattering effects. These measurements provide new insight into the underlying mechanisms and theoretical modeling of jet quenching.

PHYSICAL REVIEW LETTERS 135[3], 031901, 2025. DOI: 10.1103/PhysRevLett.135.031901. Acesso: <https://doi.org/10.1103/PhysRevLett.135.031901>

[P357-2025] “Search for rare decays of the Z and Higgs bosons to a J/ψ or $\psi(2S)$ meson and a photon in proton-proton collisions at $\sqrt{s}=13$ TeV”

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

A search is presented for rare decays of the Z and Higgs bosons to a photon and a J/ψ or a $\psi(2S)$ meson, with the charmonium state subsequently decaying to a pair of muons. The data set corresponds to an integrated luminosity of 123 fb⁻¹ of proton-proton collisions at a center-of-mass energy of 13 TeV collected with the CMS detector at the LHC. No evidence for branching fractions of these rare decay channels larger than predicted in the standard model is observed. Upper limits at 95% confidence level are set: $B(H \rightarrow J/\psi \gamma) < 2.6 \times 10^{-4}$, $B(H \rightarrow \psi(2S)\gamma) < 9.9 \times 10^{-4}$, $B(Z \rightarrow J/\psi \gamma) < 0.6 \times 10^{-6}$, and $B(Z \rightarrow \psi(2S)\gamma) < 1.3 \times 10^{-6}$. The ratio of the Higgs boson coupling modifiers

$\kappa(c)/\kappa(\gamma)$ is constrained to be in the interval (-157, +199) at 95% confidence level. Assuming $\kappa(\gamma) = 1$, this interval becomes (-166, +208).

PHYSICS LETTERS B 865, 139462, 2025. DOI: 10.1016/j.physletb.2025.139462. Acesso: <https://doi.org/10.1016/j.physletb.2025.139462>

[P358-2025] “Security of device-independent quantum key distribution via monogamy relations from multipartite information causality”

Pollyceno, L.*; Chaturvedi, A.; Raj, C.; Dieguez, P. R.; Pawłowski, M.

The information causality principle (IC) was originally proposed as a promising means to understand the extent of quantum nonlocality without invoking the full mathematical formalism of quantum theory. Beyond the foundational significance, the problem of bounding nonlocal correlations by reasonable physical principles has meaningful practical consequences, particularly for device-independent (DI) cryptographic security. In this work, we advance in this direction, demonstrating that the IC is enough to ensure DI security on quantum key distribution (QKD) protocols. Security is proven for a range of theoretically quantum-attainable parameters against individual attacks by a potentially postquantum eavesdropper. This result follows as a consequence of a strong form of monogamy of Bell's inequality violations, which we prove to be implied by the recently proposed multipartite formulation for IC. Additionally, we demonstrate that the original bipartite formulation of IC fails to imply monogamy relations, and hence, ensure security of DIQKD, thus stressing the necessity of the multipartite framework.

PHYSICAL REVIEW A 112[4], 042201, 2025. DOI: 10.1103/jnng-m87v. Acesso: <https://doi.org/10.1103/jnng-m87v>

[P359-2025] “Site Preferences of Copper and Cobalt Monobenzo Porphyrins in a Trans-Dibenzo Adsorption Structure on Cu(111)”

Shaker, M.; Muth, M.; Steffen, J.; Ceccatto, A.; Gazetas, P.; Oleszak, C.; Siervo, A. de*; Jux, N.; Görling, A.; Steinrück, H.; Lytken, O.

Using scanning tunneling microscopy, Cu and Co tetraphenyl monobenzo porphyrins are used as probe molecules to better understand the T-type interactions within well-ordered islands of Cu and Co tetraphenyl trans-dibenzo porphyrins on Cu(111). The islands are made up of molecular rows, held together by T-type interactions between isoindole and phenyl rings of adjacent molecules. The monobenzo molecules are found to be depleted within the bulk of the molecular rows and enriched at the edges terminating the rows. By counting over 50 000 molecules and using equilibrium considerations, the T-type interaction energies within the trans-dibenzo islands are estimated and the derived values are compared to values previously calculated with density functional theory, which find very good agreement for Cu-TPtdBP but less satisfying agreement for Co-TPtdBP.

CHEMPHYSICHEM 26[22], 2025. DOI: 10.1002/cphc.202500524 Early Access Date: OCT 2025. Acesso: <https://doi.org/10.1002/cphc.202500524>

[P360-2025] “Sodium-decorated P-C3N: A porous 2D framework for high-capacity and reversible hydrogen storage”

Laranjeira, J. A. S.; Martins, N. F.; Lima, K. A. L.*; Xiao, L. T.; Chen, X. H.; Ribeiro Jr., L. A.; Sambrano, J. R.

The development of reversible hydrogen storage materials has

become crucial for enabling carbon-neutral energy systems. Based on this, the present work investigates the hydrogen storage on the sodium-decorated P-C3N (Na@P-C3N), a porous carbon nitride monolayer recently proposed as a stable semiconductor. First-principles calculations reveal that Na atoms preferentially adsorb with an adsorption energy of 4.48 eV, effectively suppressing clusterization effects. Upon decoration, the system becomes metallic, while ab initio molecular dynamics simulations confirm the thermal stability of Na@P-C3N at 300 K. Hydrogen adsorption on Na@P-C3N occurs through weak physisorption, with energies ranging from 0.18 to 0.28 eV, and desorption temperatures between 231 and 357 K. The system can stably absorb 16 H₂ molecules per unit cell, corresponding to a gravimetric storage capacity of 9.88 wt%, surpassing the U.S. Department of Energy target. These results demonstrate that Na@P-C3N is a promising candidate for lightweight, stable, and reversible hydrogen storage.

MATERIALS TODAY COMMUNICATIONS 48, 113414, 2025. DOI: 10.1016/j.mtcomm.2025.113414. Acesso: <https://doi.org/10.1016/j.mtcomm.2025.113414>

[P361-2025] “Spray-Coated Melanin/PEDOT:PSS Films for Sustainable Organic Electrochemical Transistors”

Nozella, N. L.; Nogueira, G. L.; Paulin, J. V.; Oliveira, R. F. De*; Graeff, C. F. O.

A simple and scalable protocol for the fabrication of Melanin/ PEDOT:PSS organic electrochemical transistors (OECTs) via spray coating is presented. The method includes melanin synthesis, blending with poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) PEDOT:PSS at different mass ratios (0, 10, 30, and 50 wt%, named Pure PEDOT:PSS, 10Mel, 30Mel, and 50Mel, respectively), and deposition onto gold-patterned substrates using a 3D printer-adapted spray-coating system. Electrical characterization is performed using a top-gate Ag/AgCl electrode in 100 mM NaCl aqueous electrolyte, with output and transfer curves recorded. Addition of 10 wt% melanin increases the normalized transconductance by approximately 2x compared to pristine PEDOT:PSS, while maintaining a high ON/OFF current ratio (>100). Threshold voltage shifts toward more negative potential, reflecting dedoping effects and the influence of melanin on device operation. Film morphology and thickness were systematically evaluated, providing insights into reproducibility across different compositions. This protocol enables the production of sustainable, high-performance OECTs for bioelectronic applications such as sensors, memory devices, and neuromorphic-inspired systems.

JOVE-JOURNAL OF VISUALIZED EXPERIMENTS [224], e69354, 2025. DOI: 10.3791/69354. Acesso: <https://app.jove.com/t/69354/spray-coated-melaninpedotpss-films-for-sustainable-organic>

[P362-2025] “Tailoring Pt-Based Organometallic Porous Network on Ag(111): A Model System for “Host-Guest” Chemistry”

Carreno-Diaz, V.*; Ceccatto, A.*; Ferreira, E. B. da C.*; Shaker, M.; Steinruck, H. P.; Siervo, A. de*

Metal-organic frameworks (MOFs) have proven to be versatile platforms for anchoring individual metal atoms, which can act as single-atom catalysts. Due to their well-defined geometric and electronic structure, high porosity, and adjustable pore size, MOFs can modulate the catalytic performance of anchored individual atoms. In this work, we explored the surface-assisted synthesis of 2D surface metal-organic networks (SMONs) of 1,3,5-tris[4-(pyridine)-[1,1'-biphenyl]benzene] (TPyPPB) coordinated with Pt atoms on Ag(111) by using scanning tunneling microscopy at room temperature. The Pt deposition was performed in two routes: (i) by using the

dichloro-(1,10-phenanthroline)-platinum(II) (Cl₂PhPt) or (ii) by direct deposition of Pt atoms. Using Cl₂PhPt as a Pt source and applying various annealing sequences at a temperature of 400 K, a long-range hexagonal SMONs is obtained. After the dechlorination of the Cl₂PhPt molecule, individual Pt atoms establish quadruple coordination with two N atoms at the pyridyl end groups of the TPyPPB molecule and two Cl atoms. These pores have efficiently induced the formation of large molecules that behave like rotors. Such a system has the potential to open new frontiers and shed light on a better understanding of the physical-chemistry mechanisms involved in “host-guest” chemistry.

ACS NANOSCIENCE AU, 2025. DOI: 10.1021/acsnanoscienceau.5c00124. Early Access Date: NOV 2025. Acesso: <https://doi.org/10.1021/acsnanoscienceau.5c00124>

[P363-2025] “The need for a nonlocal expansion in general relativity”

Galoppo, M.; Torrieri, G.*

Motivated by known facts about effective field theory and non-Abelian gauge theory, we argue that the post-Newtonian approximation might fail even in the limit of weak fields and small velocities for wide-extended rotating bodies, where angular momentum spans significant spacetime curvature. We construct a novel dimensionless quantity that samples this breakdown, and we evaluate it by means of existing analytical solutions of rotating extended bodies and observational data. We give estimates for galaxies and binary systems, as well as our home in the Cosmos, Laniakea. We thus propose that a novel effective field theory of general relativity might be needed to account for the onset of nonlocal angular momentum effects.

ANNALS OF PHYSICS 484, 170293, 2025. DOI: 10.1016/j.aop.2025.170293. Acesso: <https://doi.org/10.1016/j.aop.2025.170293>

[P364-2025] “The quantum Newton’s bucket: Active and passive rotations in quantum theory”

Facundes, A.*; Gonçalves, K. J.*; Torrieri, G.*

Motivated both by classical physics problems associated with “Newton’s bucket” and recent developments related to QCD in rotating frames of reference relevant to heavy ion collisions, we discuss the difference between “active” and “passive” rotations in quantum systems. We examine some relevant potentials and give general symmetry arguments to give criteria where such rotations give the same results. We close with a discussion of how this can be translated to problems of current interest in quantum field theory and quantum gravity.

MODERN PHYSICS LETTERS A, 2025. DOI: 10.1142/S0217732325400012 Early Access Date: DEC 2025. Acesso: <https://doi.org/10.1142/S0217732325400012>

[P365-2025] “The scintillator surface detector of the Pierre Auger observatory”

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

Data collected so far by the Pierre Auger Observatory have enabled major advances in ultra-high energy cosmic ray physics and demonstrated that improved determination of masses of primary cosmic-ray particles, preferably on an event-by-event basis, is necessary for understanding their origin and nature. Improvement in primary mass

measurements was the main motivation for the upgrade of the Pierre Auger Observatory, called AugerPrime. As part of this upgrade, scintillator detectors are added to the existing water-Cherenkov surface detector stations. By making use of the differences in detector response to the electromagnetic particles and muons between scintillator and water-Cherenkov detectors, the electromagnetic and muonic components of cosmic-ray air showers can be disentangled. Since the muonic component is sensitive to the primary mass, such combination of detectors provides a powerful way to improve primary mass composition measurements over the original Auger surface detector design. In this paper, the so-called Scintillator Surface Detectors are discussed, including their design characteristics, production process, testing procedure and deployment in the field.

JOURNAL OF INSTRUMENTATION 20[8], P08002, 2025. DOI: 10.1088/1748-0221/20/08/P08002. Acesso: <https://iopscience.iop.org/article/10.1088/1748-0221/20/08/P08002>

[P366-2025] “Two-dimensional T-C₃N functionalized with sodium: A promising platform for solid-state hydrogen storage”

Laranjeira, J. A. S.; Martins, N. F.; Aparicio-Huacarpuma, B. D.; Lima, K. A. L.*; Ribeiro J., L. A.; Sambrano, J. R.

We report a comprehensive first-principles investigation of the two-dimensional carbon nitride monolayer T-C₃N, focusing on its potential as a hydrogen storage material through sodium decoration. The pristine T-C₃N structure exhibits a porous framework with an indirect band gap of 1.61 eV. Upon Na decoration, charge redistribution and metallic character are observed, which promote the adsorption of H₂ molecules via van der Waals interactions. Na@T-C₃N achieves a maximum storage capacity of 10.63 wt% with 16 adsorbed H₂ molecules and average binding energies between -0.18 and -0.11 eV. Ab initio molecular dynamics simulations confirm the thermal stability of the system, with Na atoms remaining anchored and partial desorption of H₂ at 300 K, indicating favorable reversibility.

PHYSICA B-CONDENSED MATTER 719, 417945, 2025. DOI: 10.1016/j.physb.2025.417945. Acesso: <https://doi.org/10.1016/j.physb.2025.417945>

[P367-2025] “Uniaxial stress tuning of the anomalous Hall effect in Mn₃Ge”

Lombardi, G. A.*; Kutelak, L. O.*; Piva, M. M.; Frehse, V. E. S.*; Calligaris, G. A.; Manna, K.; Felser, C.; Reis, R. D. Dos; Nicklas, M.

Tunable electronic properties in magnetic materials lead to novel physical phenomena that have the potential to be exploited in the design of new spintronic devices. Here, we report the effect of uniaxial stress on the anomalous Hall effect (AHE) in the hexagonal frustrated antiferromagnetic Heusler compound Mn₃Ge. Our x-ray diffraction results show that the c/a ratio varies linearly with strain when stress is applied along the a axis, as well as a significantly higher Young’s modulus along the c direction. The linear behavior of the c/a ratio under uniaxial stress mirrors that seen under hydrostatic pressure up to 1.8 GPa, but results in a characteristically different behavior of the AHE. Stress applied along the a axis induces a distortion in the ab plane, smoothing the abrupt jump in the AHE signal at zero magnetic field. In contrast, stress applied along the c axis has little effect, presumably due to the higher Young’s modulus. We argue that this is due to pronounced changes in magnetic order.

PHYSICAL REVIEW MATERIALS 9[10], 104204, 2025. DOI: 10.1103/k1c5-cs6g. Acesso: <https://doi.org/10.1103/k1c5-cs6g>

[P368-2025] “Unraveling Mn intercalation and diffusion in

NbSe₂ bilayers through DFTB simulations”

Ipaves, B.*; Oliveira, R. B. de; Fabris, G. da S. L.*; Batzill, M.; Galvao, D. S.*

Understanding transition metal atoms' intercalation and diffusion behavior in two-dimensional (2D) materials is essential for optimizing their performance in emerging applications. In this study, we used density functional tight binding (DFTB) simulations to investigate the atomic-scale mechanisms of manganese (Mn) intercalation into NbSe₂ bilayers. Our results show that Mn prefers intercalated and embedded positions rather than surface adsorption, as cohesive energy calculations indicate enhanced stability in these configurations. Nudged elastic band (NEB) calculations revealed an energy barrier of 0.68 eV for the migration of Mn into the interlayer, comparable to other substrates, suggesting accessible diffusion pathways. Molecular dynamics (MD) simulations further demonstrated an intercalation concentration-dependent behavior. Mn atoms initially adsorb on the surface and gradually diffuse inward, resulting in an effective intercalation at higher Mn densities before clustering effects emerge. These results provide helpful insights into the diffusion pathways and stability of Mn atoms within NbSe₂ bilayers, consistent with experimental observations and offering a deeper understanding of heteroatom intercalation mechanisms in transition metal dichalcogenides.

PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES 175, 116355, 2025. DOI: 10.1016/j.physe.2025.116355. Acesso: <https://doi.org/10.1016/j.physe.2025.116355>

[P369-2025] “Unstable mode and the Unruh-DeWitt detector”

Felipe, B. S.*; Pitelli, J. P. M.

We investigate the quantization of a single unstable mode in a real scalar field subject to a Robin boundary condition in (1+1)-dimensional half-Minkowski spacetime. The instability arises from an imaginary frequency mode—analogue to that of the inverted harmonic oscillator—requiring the rigged Hilbert space formalism for consistent quantization. Within this framework, the unstable mode is naturally described as a well-defined decaying (or growing) quantum state with a characteristic mean lifetime. We investigate its physical consequences via the response of an Unruh-DeWitt detector along static, inertial, and uniformly accelerated trajectories. For static and inertial observers, the detector response exhibits a Breit-Wigner resonance profile, with a decay width determined by the unstable frequency and a Doppler factor. In the Neumann limit, infrared divergences emerge from arbitrarily low-frequency modes. Interestingly, for accelerated detectors, the response acquires a nontrivial dependence on acceleration, and the Neumann limit yields a finite, oscillatory signal rather than a divergence, suggesting that acceleration can act as an effective infrared regulator.

Physical review. D, Covering particles, fields, gravitation, and cosmology 112[8], 085027, p. 1-12, 2025. DOI: 10.1103/physrevd.112.085027. Acesso: <https://journals.aps.org/prd/abstract/10.1103/physrevd.112.085027>

[P370-2025] “ α -, β -, and γ -TODD-G: Novel 2D planar carbon allotropes”

Lima, K. A. L.*; Laranjeiras, J. A. S.; Silva, A. M. A.; Aparicio-Huacarpuma, B. D.; Vasconcelos, F. M.; Sambrano, J. R.; Galvao, D. S.*; Ribeiro Jr., L. A.

We report a comprehensive first-principles investigation of three novel two-dimensional carbon allotropes: α -, β -, and γ -TODD-G (TODD-G), composed of 3-8-12-16, 3-8-12-16, and 3-4-8-12 interconnected carbon rings with sp² hybridization, respectively. Structural optimization, phonon spectra, and ab initio

molecular dynamics confirm their thermal and dynamic stability. All phases exhibit metallic electronic character, with distinct Dirac-like features and tilted Dirac cones suggesting anisotropic charge transport. Mechanical analysis reveals tunable anisotropy: α -TODD-G is strongly anisotropic, β -TODD-G displays moderate anisotropy, and γ -TODD-G shows near-isotropic mechanical response. Optical spectra further distinguish the phases, with γ -TODD-G showing pronounced absorption in the infrared, while α - and β -TODD-G absorb mainly in the visible and UV regions.

COMPUTATIONAL CONDENSED MATTER 45, e01154, 2025. DOI: 10.1016/j.cocom.2025.e01154. Acesso: <https://doi.org/10.1016/j.cocom.2025.e01154>

[P371-2025] “ α -Pinene and β -Pinene as Natural Adjuvants Against MRSA: Evidence from in vivo Models and Molecular Docking”

Barros, A. V. de; Veras, B. O. de; Menezes, G. D.; Bezerra, K. S.*; Mendes, R. F. V.; Santos, P. É. M. dos; Ximenes, R. M.; Fulco, U. L.; Galvao, D. S.*; Paiva, P. M. G.; Silva, M. V. da; Coutinho, H. D. M.; Oliveira, M. B. M. de

Staphylococcus aureus is a major pathogen in Healthcare-Associated Infections (HAIs), with antibiotic resistance and virulence factors that hinder treatment and reduce therapeutic options. Natural terpenes such as α -pinene (APN) and β -pinene (BPN) have emerged as potential modulators of bacterial resistance. This study assessed the antibacterial and antivirulence activities of APN and BPN, alone and in combination with antibiotics, against S. aureus. The Minimum Inhibitory Concentrations (MICs) of the selected terpenes and antibiotics were defined by the broth microdilution method, and synergistic interactions were determined by checkerboard assays, followed by growth kinetics, time-kill curves, and antivirulence assays targeting biofilm formation, coagulase activity, and hemolysin production. In vivo toxicity, bacterial burden, and host survival were evaluated using the Galleria mellonella model. Both compounds exhibited MICs ranging from 64 to 4,096 μ g/mL, with BPN showing pronounced synergy with amoxicillin (BPA) and oxacillin (BPO). The BPO combination reduced bacterial load by 82.1% and more effectively inhibited virulence factors than APN. In silico analyses supported these findings, revealing strong interactions between pinenes and key bacterial targets. No toxicity was observed in vivo. These results highlight BPN as a promising adjuvant candidate to enhance β -lactam efficacy against S. aureus, supporting integrated antibacterial and antivirulence strategies.

CURRENT MICROBIOLOGY 83[1], 19, 2025. DOI: 10.1007/s00284-025-04593-4. Acesso: <https://doi.org/10.1007/s00284-025-04593-4>

Eventos publicados

[P372-2025] “Hybrid integration of 2D dichalcogenides for low power saturable absorption in photonic integrated circuits”

Volpato, M. C.*; Magro, G. H.*; Barea, L. A. M.; Assis, P. L. de*; Frateschi, N. C.*
IEEE

Low power nonlinear behavior is needed for photonic neural networks. The incorporation of 2D transition metal dichalcogenides crystals, in particular, films with single 1T'-MoTe₂ layer onto integrated photonics structure is modeled and demonstrated for achieving ultra-low absorption saturation power in silicon nitride based structures.

PHOTONICS NORTH, PN, Série de livros: Photonics North, 2025. DOI: 10.1109/PN66844.2025.11097089. Acesso: <https://ieeexplore.ieee.org/document/11097089>

[P373-2025] "Spectrum-based alignment of SIRIUS undulators"

Ascensão, G. R.*; Liu, L.*; Luiz, S. A. L.

In-vacuum insertion devices have their magnets positioned just a few millimeters from the electron beam orbit. Due to this proximity, the emitted radiation spectrum is highly sensitive to misalignments of the device's magnetic center. Such misalignments can lead to photon flux losses, spectral shifts toward lower energies, and harmonic bandwidth broadening. This work presents the application of a spectrum-based alignment method to one of the new SIRIUS insertion devices, aiming to optimize its spectral performance at the beamline.

Journal of Physics: Conference Series 3094, 012011, 2025. DOI: 10.1088/1742-6596/3094/1/012011.

Acesso: <https://iopscience.iop.org/article/10.1088/1742-6596/3094/1/012011>

Artigos que foram destaque de capa

[Publicado no boletim de agosto] "Magnetically Tunable Polariton Cavities in van der Waals Heterostructures"

Mayer, R. A.*; Chen, X. Z.; Jing, R.; Tsuneto, M.; Zhou, B. Y.; Zhou, Z. J.; Zheng, W. J.; Pu, R.; Xu, S. H.; Liu, T.; Yao, H. L.; Wehmeier, L.; Dong, Y. N.; Sun, D. H.; He, L.; Cadore, A. R.; Heinz, T.; Fan, J. A.; Dean, C. R.; Basov, D. N.; Du, X.; Freitas, R. O.; Liu, M. K.

NANO LETTERS, 2025. Acesso em: <https://doi.org/10.1021/acs.nanolett.5c02168>. Early Access Date: JUL 2025 (Artigo destaque de capa)

[Publicado no boletim de outubro] "Reciprocating thermal behavior and thermometry studies of Tb³⁺- and Gd³⁺-oxamate single-ion magnets"

Araujo Junior, C. R.; Murad, L. M.; Perrella, R. V.; Oliveira, W. X. C.; Pinheiro, C. B.; Ramos, T. F.; Patricio, P. S. O.; Pedroso, E. F.; Nunes, W. C.; Ribeiro, P. R. T.*; Muraca, D.*; Fabris, F.*; Knobel, M.*; Sigoli, F. A.; Pereira, C. L. M.

INORGANIC CHEMISTRY FRONTIERS, 2025. DOI: 10.1039/d5qi01603g Early Access Date: SEP 2025. Acesso: <https://doi.org/10.1039/D5QI01603G>. (Artigo destaque de capa)

*Autores da comunidade IFGW

Fonte: Web of Science on-line (WOS)

Defesas de dissertações do IFGW

[D019-2025] "Tensão das constantes cosmológicas H_0 e σ_8 "

Aluno: Felipe Alberto Butzke

Orientador: Profa. Dra. Flávia Sobreira

Data: 03/12/2025

[D020-2025] "Geração de Feixes de Raios X com Momento Angular Orbital no Sirius"

Aluno: Regis Schiavon de Oliveira

Orientador: Prof. Dr. Tulio Costa Rizuti da Rocha

Data: 05/12/2025

[D021-2025] "Importância das Interações de Estado Final para Geração de Violação de CP nos Decaimentos $D^0 \rightarrow \pi\pi$, $D^0 \rightarrow KK$ e $D^0 \rightarrow \eta\eta$ "

Aluno: Cauê Piccollo Comparini

Orientador: Profa. Dra. Patrícia Camargo Magalhães

Data: 09/12/2025

[D022-2025] "Caracterização do Background de Nêutrons na Detecção de Neutrinos com Paleo-detectores"

Aluno: Matheus Santos de Sá Bergamo

Orientador: Prof. Dr. Sandro Guedes de Oliveira

Data: 12/12/2025

[D023-2025] "Interações multi-fotônicas e multi-excitônicas em pontos quânticos de perovskita: um estudo sobre ganho óptico"

Aluno: Bethânia Albuquerque Gomes

Orientador: Prof. Dr. Lázaro Aurélio Padilha Júnior

Data: 16/12/2025

Defesas de teses do IFGW

[T019-2025] "Manipulação de complexos excitônicos em monocamadas e heteroestruturas de WSe₂ usando ondas acústicas de superfície"

Aluno: Marcos Luiz Ferreira Gomes

Orientador: Prof. Dr. Odilon Divino Damasceno Couto Junior

Data: 10/12/2025

[T020-2025] "Efeitos da Pressão Hidrostática e Tensão Uniaxial em Materiais com Topologia Não Trivial"

Aluno: Leonardo Oparacz Kutelak

Orientador: Prof. Dr. Ricardo Donizeth dos Reis

Data: 10/12/2025

[T021-2025] "Study of Crystalline Electric Field effects in low-symmetry Ce-based compounds"

Aluno: Ana Maria Caffer

Orientador: Prof. Dr. Pascoal José Giglio Pagliuso

Data: 17/12/2025

Fonte: Portal IFGW/Eventos

Disponível em: [https://portal.ifi.unicamp.br/a-instituicao/eventos/month.calendar/2025/12/16/-](https://portal.ifi.unicamp.br/a-instituicao/eventos/month.calendar/2025/12/16/)

Abstracta

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