

# Abstracta

Ano XXI - N. 05

Out-17



Artigos publicados - P188-2017 à P234-2017

Correções - Co002-2017 à Co003-2017

Defesas de Teses do IFGW - T018-2017

Patentes - Pa003-2017 à Pa004-2017

## Artigos publicados

### [P188-2017] "A Bi-Sheath Fiber Sensor for Giant Tensile and Torsional Displacements"

Wang, R.; Jiang, N.; Su, J.; Yin, Q.; Zhang, Y.; Liu, Z.; Lin, H.; Moura, F. A.\*; Yuan, N.; Roth, S.; Rome, R. S.; Ovalle-Robles, R.; Inoue, K.; Yin, S.; Fang, S.; Wang, W.; Ding, J.; Shi, L.; Baughman, R. H.; Liu, Z.

Current research about resistive sensors is rarely focusing on improving the strain range and linearity of resistance-strain dependence. In this paper, a bi-sheath buckled structure is designed containing buckled carbon nanotube sheets and buckled rubber on rubber fiber. Strain decrease results in increasing buckle contact by the rubber interlayer and a large decrease in resistance. The resulting strain sensor can be reversibly stretched to 600%, undergoing a linear resistance increase as large as 102% for 0-200% strain and 160% for 200-600% strain. This strain sensor shows high linearity, fast response time, high resolution, excellent stability, and almost no hysteresis.

ADVANCED FUNCTIONAL MATERIALS 27[35], 1702134, 2017. DOI: 10.1002/adfm.201702134

### [P189-2017] "Analysis of zero field and field cooled magnetization curves of CoFe2O4 nanoparticles with a T-dependence on the saturation magnetization"

Peixoto, E. B.; Carvalho, M. H.; Meneses, C. T.; Sarmento, V. H. V.; Coelho, A. A.\*; Zucolotto, B.; Duque, J. G. S.\*

In this work, CoFe<sub>2</sub>O<sub>4</sub> nanoparticles embedded inside an amorphous SiO<sub>2</sub> were produced by the sol-gel method through the hydrolysis and condensation of tetraethyl orthosilicate (TEOS). In order to improve the sample homogeneity, a set of samples was prepared for using citric acid. Morphological and magnetic properties have been obtained via transmission electronic microscopy (TEM) and AC and DC magnetization measurements, respectively. TEM analysis indicate that nanoparticles present a spherical-like shape. The broad peaks and the presence of thermal hysteresis at low temperatures in the Zero-Field Cooled and Field-Cooled (ZFC/FC) curves are consistent with the superparamagnetism phenomenon. Once the maximum magnetization,  $M(H = 70 \text{ kOe})$ , extracted from the  $M$  vs  $H$  loops is not constant along the studied temperature range we have used, for the first time, a T-dependence of the saturation magnetization,  $M_s$ , to fit the ZFC/FC magnetization curves. Finally, the extracted parameter from both ZFC/FC magnetization curves and AC susceptibilities fits are used to calculate the nanoparticles mean sizes. These results are in good agreement with that extracted from transmission electronic microscopy.

JOURNAL OF ALLOYS AND COMPOUNDS 721, 525-530, 2017. DOI: 10.1016/j.dallcom.2017.05.246

### [P190-2017] "Anderson localization of composite excitations in disordered optomechanical arrays"

Roque, T. F.\*; Peano, V.; Yevtushenko, O. M.; Marquardt, F.

Optomechanical (OMA) arrays are a promising future platform for studies of transport, many-body dynamics, quantum control and topological effects in systems of coupled photon and phonon modes. We introduce disordered OMA arrays, focusing on features of Anderson localization of hybrid photon-phonon excitations. It turns out that these represent a unique disordered system, where basic parameters can be easily controlled by varying the frequency and the amplitude of an external laser field.

We show that the two-species setting leads to a non-trivial frequency dependence of the localization length for intermediate laser intensities. This could serve as a convincing evidence of localization in a non-equilibrium dissipative situation.

NEW JOURNAL OF PHYSICS 19, 013006, 2017. DOI: 10.1088/1367-2630/aa52e2

### [P191-2017] "Anisotropic elastic modulus, high Poisson's ratio and negative thermal expansion of graphynes and graphdiynes"

Hernandez, S. A.\*; Fonseca, A. F.\*

Graphyne (GY) and graphdiyne (GDY) are two-dimensional one-atom-thick carbon allotropes highly considered to substitute graphene in electronic applications because of the prediction of non-null band-gap. There are multiple configurations of GY structures not yet fully investigated in literature. In this work, by means of classical molecular dynamics simulations, the Young's modulus, Poisson's ratio and linear thermal expansion coefficient (TEC) of all originally proposed seven types of GYs and corresponding GDYs are calculated. The dependence of these properties with the density of the structure is investigated for the first time. Quadratic increasing of the TEC of GY and GDY structures with density was found. The elastic modulus of GYs and GDYs were shown to be more sensitive to their density than general porous materials. In particular, non-symmetric structures are much softer along the armchair direction than along zigzag direction, implying that the elasticity along armchair direction of GY and GDY structures are similar to that of porous gels materials. Values larger than unity were found for the Poisson's ratio of some non-symmetric GYs and GDYs. A simple honeycomb mechanical model is shown to capture the observed values of Poisson's ratio of GYs and GDYs.

DIAMOND AND RELATED MATERIALS 77, 57-64, 2017. DOI: 10.1016/j.diamond.2017.06.002

### [P192-2017] "Anomalous Evolution of the Near-Side Jet Peak Shape in Pb-Pb Collisions at root S-NN=2.76 TeV"

Adam, J.; Adamova, D.; Aggarwal, M. M.; Albuquerque, D. S. D.\*; Chinellato, D. D.\*; De Souza, R. D.\*; Takahashi, J.\*; et al. ALICE Collaboration

The measurement of two-particle angular correlations is a powerful tool to study jet quenching in a  $p(T)$  region inaccessible by direct jet identification. In these measurements pseudorapidity ( $\Delta\eta$ ) and azimuthal ( $\Delta\phi$ ) differences are used to extract the shape of the near-side peak formed by particles associated with a higher  $p(T)$  trigger particle ( $1 < p(T, \text{trig}) < 8 \text{ GeV}/c$ ). A combined fit of the near-side peak and long-range correlations is applied to the data allowing the extraction of the centrality evolution of the peak shape in Pb-Pb collisions at  $\sqrt{s(\text{NN})} = 2.76 \text{ TeV}$ . A significant broadening of the peak in the  $\Delta\eta$  direction at low  $p(T)$  is found from peripheral to central collisions, which vanishes above  $4 \text{ GeV}/c$ , while in the  $\Delta\phi$  direction the peak is almost independent of centrality. For the 10% most central collisions and  $1 < p(T, \text{assoc}) < 2 \text{ GeV}/c$ ,  $1 < p(T, \text{trig}) < 3 \text{ GeV}/c$  a novel feature is observed: a depletion develops around the center of the peak. The results are compared to pp collisions at the same center of mass energy and AMPT model simulations. The comparison to the investigated models suggests that the broadening and the development of the depletion is connected to the strength of radial and longitudinal flow.

PHYSICAL REVIEW LETTERS 119[10], 102301, 2017. DOI: 10.1103/PhysRevLett.119.102301



[P193-2017] "Atomic pair distribution function at the Brazilian Synchrotron Light Laboratory: application to the Pb<sub>1-x</sub>LaxZr<sub>0.40</sub>Ti<sub>0.60</sub>O<sub>3</sub> ferroelectric system"

Saleta, M. E.\*; Eleoterio, M.; Mesquita, A.; Mastelaro, V. R.; Granado, E.\*

This work reports the setting up of the X-ray diffraction and spectroscopy beamline at the Brazilian Synchrotron Light Laboratory for performing total scattering experiments to be analyzed by atomic pair distribution function (PDF) studies. The results of a PDF refinement for Al<sub>2</sub>O<sub>3</sub> standard are presented and compared with data acquired at a beamline of the Advanced Photon Source, where it is common to perform this type of experiment. A preliminary characterization of the Pb<sub>1-x</sub>LaxZr<sub>0.40</sub>Ti<sub>0.60</sub>O<sub>3</sub> ferroelectric system, with  $x = 0.11, 0.12$  and  $0.15$ , is also shown.

JOURNAL OF SYNCHROTRON RADIATION 24, 1098-1104, Part: 5, 2017. DOI: 10.1107/S1600577517008633

[P194-2017] "Characterization of PECVD a-C:H:Si:O:Cl films"

Rossi, D.; Landers, R.\*; Bortoleto, J. R. R.; Durrant, S. F.

Thin films were produced by plasma enhanced chemical vapor deposition of tetramethylsilane, chloroform, and argon mixtures. The partial pressure of chloroform in the chamber feed, CCl<sub>4</sub>, was varied from 0% to 40%. Amorphous hydrogenated carbon films also containing silicon, oxygen, and small amounts of chlorine, a-C: H: Si: O: Cl, were produced at deposition rates of up to about 220 nm min<sup>-1</sup> (for a CCl<sub>4</sub> of 40%). Transmission infrared analyses revealed the presence of OH groups in chlorinated films, along with, among others, CH, C-C, Si-CH, Si-CH<sub>2</sub>, and Si-O-Si groups. As revealed by energy dispersive x-ray spectroscopy, the films could be doped with chlorine to a maximum of about 3 at. %. Surface morphology and roughness were examined using scanning electron microscopy and atomic force microscopy. Tauc band gaps, calculated from transmission ultraviolet-visible near infrared spectra, tend to decrease from similar to 3.4 eV for unchlorinated films to around 2.5 eV for those doped with chlorine.

JOURNAL OF VACUUM SCIENCE & TECHNOLOGY A 35[4], SI, 04D103, 2017. DOI: 10.1116/1.4982711

[P195-2017] "Characterizing Slow Photochemical Reaction Kinetics by Enhanced Sampling of Rare Events with Capillary Optical Fibers and Kramers' Theory"

Nome, R. A.; Costa, A. F.; Lepkoski, J.; Monteiro, G. A.; Hayashi, J. G.\*; Cordeiro, C. M. B.\*

Characterization of slow chemical reactions is essential for assessing catalytic efficiency in chemistry and biology. [GRAPHIC] Traditionally, chemical reaction rates are obtained from population relaxation kinetics measurements and the Arrhenius equation. Unfortunately, it is difficult to use this approach to characterize reactions wherein concentrations change slowly. Thus, it is interesting to see whether a dynamical view of chemical reactions may be used to obtain the reaction rates of slow processes. In the present work, we perform Brownian dynamics simulations of an asymmetric double-well potential to investigate how enhanced sampling of barrier crossing at transition states improves the characterization of reaction rate constants. We then present the design of a liquid-filled capillary optical fiber-based fluorescence spectrometer, which, like rare events, is also based on Poissonian statistics. We use the instrument to characterize the slow photochemical degradation kinetics of poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV) in *o*-dichlorobenzene. We have employed in situ optical microscopy measurements and electrostatics simulations to characterize the excitation beam profile inside a liquid-filled capillary fiber.

We compare the cuvette and capillary fiber sample holders and show that the MEH-PPV fluorescence line shape is independent of the sample holder, as expected. We characterize the photochemical degradation kinetics of MEH-PPV in *o*-dichlorobenzene solutions placed in the cuvette versus that in the capillary fiber. We observe small and slow changes in the time-dependent fluorescence spectra when the degradation reaction is performed in the cuvette. On the other hand, we are able to characterize reactant-concentration decay and product-concentration buildup from the time-dependent fluorescence spectra recorded during photochemical degradation of MEH-PPV performed inside the capillary optical fiber. Ultrafast optically heterodyne-detected optical Kerr effect spectroscopy and multimode Brownian oscillator analysis provide further insights into the role of bath oscillator modes of friction in the mechanism of MEH-PPV photochemical degradation. Overall, the work presented herein shows that slow photochemical degradation kinetics of MEH-PPV can be successfully and efficiently assessed in the capillary fiber fluorescence spectrometer.

ACS OMEGA 2[6], 2719-2727, 2017. DOI: 10.1021/acsomega.7b00004

[P196-2017] "Control of entanglement dynamics in a system of three coupled quantum oscillators"

Gonzalez-Henao, J. C.\*; Pugliese, E.; Euzzor, S.; Meucci, R.; Roversi, J. A.\*; Arecchi, F. T.

Dynamical control of entanglement and its connection with the classical concept of instability is an intriguing matter which deserves accurate investigation for its important role in information processing, cryptography and quantum computing. Here we consider a tripartite quantum system made of three coupled quantum parametric oscillators in equilibrium with a common heat bath. The introduced parametrization consists of a pulse train with adjustable amplitude and duty cycle representing a more general case for the perturbation. From the experimental observation of the instability in the classical system we are able to predict the parameter values for which the entangled states exist. A different amount of entanglement and different onset times emerge when comparing two and three quantum oscillators. The system and the parametrization considered here open new perspectives for manipulating quantum features at high temperatures.

SCIENTIFIC REPORTS 7, 9957, 2017. DOI: 10.1038/s41598-017-09989-2

[P197-2017] "Core or Cusps: The Central Dark Matter Profile of a Strong Lensing Cluster with a Bright Central Image at Redshift 1"

Collett, T. E.; Buckley-Geer, E.; Lin, H.; Sobreira, F.\*; et.al.

We report on SPT-CLJ2011-5228, a giant system of arcs created by a cluster at  $z = 1.06$ . The arc system is notable for the presence of a bright central image. The source is a Lyman break galaxy at  $z(s) = 2.39$  and the mass enclosed within the Einstein ring of radius 14 arcsec is similar to  $10(14.2) M_{\odot}$ . We perform a full reconstruction of the light profile of the lensed images to precisely infer the parameters of the mass distribution. The brightness of the central image demands that the central total density profile of the lens be shallow. By fitting the dark matter as a generalized Navarro-Frenk-White profile-with a free parameter for the inner density slope-we find that the break radius is  $270(-76)(+48)$  kpc, and that the inner density falls with radius to the power  $-0.38 \pm 0.04$  at 68% confidence. Such a shallow profile is in strong tension with our understanding of relaxed cold dark matter halos; dark matter-only simulations predict that the inner density should fall as  $r^{-1}$ .

The tension can be alleviated if this cluster is in fact a merger; a two-halo model can also reconstruct the data, with both clumps (density varying as  $r(-0.8)$  and  $r(-1.0)$ ) much more consistent with predictions from dark matter-only simulations. At the resolution of our Dark Energy Survey imaging, we are unable to choose between these two models, but we make predictions for forthcoming Hubble Space Telescope imaging that will decisively distinguish between them.

**ASTROPHYSICAL JOURNAL** 843[2], 148, 2017. DOI: 10.3847/1538-4357/aa76e6

**[P198-2017] “Direct Electron Beam Writing of Silver-Based Nanostructures”**

Hoeflich, K.; Jurczyk, J.; Zhang, Y.; Puydinger dos Santos, M. V.\*; Goetz, M.; Guerra-Nunez, C.; Best, J. P.; Kapusta, C.; Utke, I.

Direct writing utilizing a focused electron beam constitutes an interesting alternative to resist-based techniques, as it allows for precise and flexible growth onto any conductive substrate in a single-step process. One important challenge, however, is the identification of appropriate precursors which allow for deposition of the material of choice, e.g., for envisaged applications in nano-optics. In this regard the coinage metal silver is of particular interest since it shows a relatively high plasma frequency and, thus, excellent plasmonic properties in the visible range. By utilizing the precursor compound  $\text{AgO}_2\text{Me}_2\text{Bu}$ , direct writing of silver-based nanostructures via local electron beam induced deposition could be realized for the first time. Interestingly, the silver deposition was strongly dependent on electron dose; at low doses of 30 nC/ $\mu\text{m}^2$  a dominant formation of pure silver crystals was observed, while at higher electron doses around 104 nC/ $\mu\text{m}^2$  large carbon contents were measured. A scheme for the enhanced silver deposition under low electron fluxes by an electronic activation of precursor dissociation below thermal CVD temperature is proposed and validated using material characterization techniques. Finally, the knowledge gained was employed to fabricate well-defined two-dimensional deposits with maximized silver content approaching 75 at. %, which was achieved by proper adjustment of the deposition parameters. The corresponding deposits consist of plasmonically active silver crystallites and demonstrate a pronounced Raman signal enhancement of the carbonaceous matrix.

**ACS APPLIED MATERIALS & INTERFACES** 9[28], 24071-24077, 2017. DOI: 10.1021/acsami.7b04353

**[P199-2017] “Enhanced properties of cement mortars with multilayer graphene nanoparticles”**

Silva, R. A. E.; Guetti, P. D.; da Luz, M. S.; Rouxinol, F.\*; Gelamo, R. V.

The present work aims to combine multilayer graphene (MLG) nanoparticles with Ordinary Portland Cement (OPC) mortar specimens, evaluating possible improvements on their mechanical properties and ultimately coming up with an ideal and effective concentration for future applications. Mortars with water/cement ratio of 0.4, MLG dosage varying from 0.015 to 0.033% by weight of cement and sand at a proportion of 3 x the weight of cement were prepared. 50 x 100 mm cylindrical specimens were shaped and subjected to compressive and splitting tensile strength tests at the ages of 3, 7 and 28 days. In addition, SEM micrographs and metallographic images were collected and analyzed in order to better characterize the sample's morphology and also in attempt of explaining the MLG influence on cement paste. The optimal tensile strength was achieved with samples designed with MLG dosage of 0.033%, for which the corresponding increases were 100.0, 144.4 and 131.6%, after 3, 7 and 28 days, respectively, compared with samples without MLG.

On the other hand, the optimal compressive strength increases were obtained with samples designed with MLG dosage of 0.021%, with improvements of 63.6, 94.1 and 95.7% after 3, 7 and 28 days, respectively, compared with samples without MLG. The addition of MLG is believed to accelerate cement hydration reactions, reduce the pore volume and harden cement properties. An improvement in thermal conductivity is also associated to MLG incorporation, and this favorable heat transfer in OPC-based mortars probably promoted the observed changes in the composite chemical structure and mechanical properties herein analyzed.

**CONSTRUCTION AND BUILDING MATERIALS** 149, 378-385, 2017. DOI: 10.1016/j.conbuildmat.2017.05.146

**[P200-2017] “Ethanol Solvation in Water Studied on a Molecular Scale by Photoelectron Spectroscopy”**

Marinho, R. R. T.; Walz, M. M.; Ekholm, V.; Ohrwall, G.; Bjorneholm, O.; de Brito, A. N.\*

Because of the amphiphilic properties of alcohols, hydrophobic hydration is important in the alcohol water system. In the present paper we employ X-ray photoelectron spectroscopy (XPS) to investigate the bulk and surface molecular structure of ethanol water mixtures from 0.2 to 95 mol %. The observed XPS binding energy splitting between the methyl C and hydroxymethyl C is groups ( $\text{BES}_{[\text{CH}_3\text{-CH}_2\text{OH}]}$ ) as a function of the ethanol molar percentage can be divided into different regions: one below 35 mol % with higher values (about 1.53 eV) and one starting at 60 mol % up to 95 mol % with 1.49 eV as an average value. The chemical shifts agree with previous quantum mechanics/molecular mechanics (QM/MM) calculations [Loytynoja, T.; et al. *J. Phys. Chem. B* 2014, 118, 13217]. According to these calculations, the  $\text{BES}_{[\text{CH}_3\text{-CH}_2\text{OH}]}$  is related to the number of hydrogen bonds between the ethanol and the surrounding molecules. As the ethanol concentration increases, the average number of hydrogen bonds decreases from 2.5 for water-rich mixtures to 2 for pure ethanol. We give an interpretation for this behavior based on how the hydrogen bonds are distributed according to the mixing ratio. Since our experimental data are surface sensitive, we propose that this effect may also be manifested at the interface. From the ratio between the XPS C 1s core lines intensities we infer that below 20 mol % the ethanol molecules have their hydroxyl groups more hydrated and possibly facing the solution's bulk. Between 0.1 and 14 mol %, we show the formation of an ethanol monolayer at approximately 2 mol %. Several parameters are derived for the surface region at monolayer coverage.

**JOURNAL OF PHYSICAL CHEMISTRY B** 121[33], 7916-7923, 2017. DOI: 10.1021/acs.jpcc.7b02382

**[P201-2017] “Evolution of the longitudinal and azimuthal structure of the near-side jet peak in Pb-Pb collisions at root  $s(\text{NN})=2.76$  TeV”**

Adam, J.; Adamova, D.; Aggarwal, M. M.; Albuquerque, D. S. D.\*; Chinellato, D. D.\*; De Souza, R. D.\*; Takahashi, J.\*; et al. ALICE Collaboration

In two-particle angular correlation measurements, jets give rise to a near-side peak, formed by particles associated to a higher- $p(\text{T})$  trigger particle. Measurements of these correlations as a function of pseudorapidity ( $\Delta\eta$ ) and azimuthal ( $\Delta\phi$ ) differences are used to extract the centrality and  $p(\text{T})$  dependence of the shape of the near-side peak in the  $p(\text{T})$  range  $1 < p(\text{T}) < 8$  GeV/c in Pb-Pb and pp collisions at root  $s(\text{NN}) = 2.76$  TeV. A combined fit of the near-side peak and long-range correlations is applied to the data and the peak shape is quantified by the variance of the distributions.

While the width of the peak in the Delta phi direction is almost independent of centrality, a significant broadening in the Delta eta direction is found from peripheral to central collisions. This feature is prominent for the low-p(T) region and vanishes above 4 GeV/c. The widths measured in peripheral collisions are equal to those in pp collisions in the Delta phi direction and above 3 GeV/c in the Delta eta direction. Furthermore, for the 10% most central collisions and  $1 < p(T, \text{assoc}) < 2$  GeV/c,  $1 < p(T, \text{trig}) < 3$  GeV/c, a departure from a Gaussian shape is found: a depletion develops around the center of the peak. The results are compared to A Multi-Phase Transport (AMPT) model simulation as well as other theoretical calculations indicating that the broadening and the development of the depletion are connected to the strength of radial and longitudinal flow.

PHYSICAL REVIEW C 96[3], 034904, 2017. DOI: 10.1103/PhysRevC.96.034904

[P202-2017] “Experimental evidence for a chiral symmetry-breaking mechanism in aspartic acid: Lattice and sub-lattice matching”

Teschke, O.\*; Soares, D. M.\*

A mother crystal formed from a transient molecular structure of (D+L) aspartic acid in solution is reported. Hexagonal structures with a lattice constant of 1.04 nm were crystallized from a solution in which three aspartic acid species coexist: right- and left-handed enantiomorphs, denoted D-aspartic and L-aspartic, respectively, and transitory (D+L) aspartic acid specie. Atomic force microscopy images of the crystalline deposits reveal domains of the transitory (D+L) aspartic acid crystal forming the substrate deposit on silicon wafers, and on top of this hexagonal lattice only L-aspartic acid is observed to conform and crystallize. A preferential crystallization mechanism is then observed for (D+L) aspartic acid crystals that seed only L-aspartic deposits by the geometrical matching of their multiple hexagonal lattice structures with periodicities of 1.04 nm and 0.52 nm, respectively.

JOURNAL OF CRYSTAL GROWTH 475, 110-114, 2017. DOI: 10.1016/j.jcrysgro.2017.06.005

[P203-2017] “Hybrid multimode resonators based on grating-assisted counter-directional couplers”

Davis, J. A.; Grieco, A.; Souza, M. C. M. M.\*; Frateschi, N. C.\*; Fainman, Y.

Research thrusts in silicon photonics are developing control operations using higher order waveguide modes for next generation high-bandwidth communication systems. In this context, devices allowing optical processing of multiple waveguide modes can reduce architecture complexity and enable flexible on-chip networks. We propose and demonstrate a hybrid resonator dually resonant at the 1st and 2nd order modes of a silicon waveguide. We observe 8 dB extinction ratio and modal conversion range of 20 nm for the 1st order quasi-TE mode input.

OPTICS EXPRESS 25[14] 16484-16490, 2017. DOI: 10.1364/OE.25.016484

[P204-2017] “Insight into particle production mechanisms via angular correlations of identified particles in pp collisions at root s=7 TeV”

Adam, J.; Adamova, D.; Aggarwal, M. M.; Albuquerque, D. S. D.\*; Chinellato, D. D.\*; De Souza, R. D.\*; Takahashi, J.\*; et al. ALICE Collaboration

Two-particle angular correlations were measured in pp collisions at root s = 7 TeV for pions, kaons, protons, and lambdas, for all particle/anti-particle combinations in the pair. Data for mesons exhibit an expected peak dominated by effects associated with mini-jets and are well reproduced by general purpose Monte Carlo generators. However, for baryon-baryon and anti-baryon-anti-baryon pairs, where both particles have the same baryon number, a near-side anti-correlation structure is observed instead of a peak. This effect is interpreted in the context of baryon production mechanisms in the fragmentation process. It currently presents a challenge to Monte Carlo models and its origin remains an open question.

EUROPEAN PHYSICAL JOURNAL C 77[8], 569, 2017. DOI: 10.1140/epjc/s10052-017-5129-6

[P205-2017] ““Inverted” porphyrins: a distorted adsorption geometry of free-base porphyrins on Cu(111)”

Lepper, M.; Koebl, J.; Schmitt, T.; Gurrath, M.; de Siervo, A.\*; Schneider, M. A.; Steinrueck, H. P.; Meyer, B.; Marbach, H.; Hieringer, W.

Based on density functional theory calculations combined with experimental results, we report and discuss an extremely distorted, “inverted” adsorption geometry of free-base tetraphenylporphyrin on Cu(111). The current findings yield new insights into a wellstudied system, shedding light on the peculiar molecule-substrate interaction and the resulting intramolecular conformation.

CHEMICAL COMMUNICATIONS 53[58], 8207-8210, 2017. DOI: 10.1039/c7cc04182a

[P206-2017] “Investigation of the leading and subleading high-energy behavior of hadron-hadron total cross sections using a best-fit analysis of hadronic scattering data”

Giordano, M.; Meggiolaro, E.; Silva, P. V. R. G.\*

In the present investigation we study the leading and subleading high-energy behavior of hadron-hadron total cross sections using a best-fit analysis of hadronic scattering data. The parametrization used for the hadron-hadron total cross sections at high energy is inspired by recent results obtained by Giordano and Meggiolaro [J. High Energy Phys. 03 (2014) 002] using a nonperturbative approach in the framework of QCD, and it reads  $\sigma_{\text{tot}} \sim B + C \ln s \ln \ln s$ . We critically investigate if B and C can be obtained by means of best-fits to data for proton-proton and antiproton-proton scattering, including recent data obtained at the LHC, and also to data for other meson-baryon and baryon-baryon scattering processes. In particular, following the above-mentioned nonperturbative QCD approach, we also consider fits where the parameters B and C are set to  $B = \kappa B_{\text{th}}$  and  $C = \kappa C_{\text{th}}$ , where  $B_{\text{th}}$  and  $C_{\text{th}}$  are universal quantities related to the QCD stable spectrum, while  $\kappa$  (treated as an extra free parameter) is related to the asymptotic value of the ratio  $\sigma_{\text{el}}/\sigma_{\text{tot}}$ . Different possible scenarios are then considered and compared.

PHYSICAL REVIEW D 96[3], 034015, 2017. DOI: 10.1103/PhysRevD.96.034015

[P207-2017] “Journeys from quantum optics to quantum technology”

Barnett, S. M.; Beige, A.; Ekert, A.; Garraway, B. M.; Keitel, C. H.; Kendon, V.; Lein, M.; Milburn, G. J.; Moya-Cessa, H. M.; Muro, M.; Pachos, J. K.; Palma, G. M.; Paspalakis, E.; Phoenix, S. J. D.; Piraux, B.; Plenio, M. B.; Sanders, B. C.; Twamley, J.; Vidiella-Barranco, A.\*; Kim, M. S.



Sir Peter Knight is a pioneer in quantum optics which has now grown to an important branch of modern physics to study the foundations and applications of quantum physics. He is leading an effort to develop new technologies from quantum mechanics. In this collection of essays, we recall the time we were working with him as a postdoc or a PhD student and look at how the time with him has influenced our research.

**PROGRESS IN QUANTUM ELECTRONICS 54[SI], 19-45, 2017.** DOI: 10.1016/j.pquantelec.2017.07.002

**[P208-2017] “Long-Range Coherent Tunneling in Physisorbed Molecular Ensembles”**

Merces, L.\*; de Oliveira, R. F.; de Camargo, D. H. S.; Bufon, C. C. B.\*

The charge transport in molecular systems is governed by a series of carrier-molecule quantum interactions, which result in a broad set of chemical and physical phenomena. The precise control of such phenomena is one of the main challenges toward the development of novel device concepts. In molecular systems, direct tunneling across 1-10 nm barriers and activated hopping over longer distances have been described as the main charge transport mechanisms. The continuous transition from one mechanism to the other, by increasing the transport distance, has mainly been reported for molecular chains covalently bonded to the electrodes. In elementary molecular junctions, like those formed by physisorbed organic semiconductor thin films, such transition remains unclear. Here, we report the first experimental evidence for sequential, long-range coherent tunneling across physisorbed ensembles by investigating the charge transport in copper phthalocyanine layers (5-60 nm thick films). Like observed for chemisorbed molecules, our junction exhibits a gradual transition from coherent tunneling to activated transport in the 10-22 nm thickness range. The present work contributes to connect the quantum transport to diffusive-related phenomena in such an elementary organic system.

**JOURNAL OF PHYSICAL CHEMISTRY C 121[31], 16673-16681, 2017.** DOI: 10.1021/acs.jpcc.7b02528

**[P209-2017] “Magnetite Nanoparticles Bonded Carbon Quantum Dots Magnetically Confined onto Screen Printed Carbon Electrodes and their Performance as Electrochemical Sensor for NADH”**

Canevari, T. C.; Cincotto, F. H.; Gomes, D.; Landers, R.\*; Toma, H. E.

Hybrid magnetite/carbon quantum dots (MagNP/C-dots) were prepared and their characterization performed by high resolution transmission electron microscopy (HR-TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). Because of their suitable magnetization and electrochemical properties, they were used as versatile electrode modifiers after magnetically confining onto screen printed carbon electrodes (SPE), with the aid of a miniature external magnet. The reported strategy introduces a convenient procedure for assembling modified electrodes, since the nanoparticles can be easily released by removing the magnet. The non-enzymatic magnetic biosensor showed excellent performance in the determination of NADH at the concentration range  $2 \times 10^{-7}$  to  $5 \times 10^{-6}$  molL<sup>-1</sup>, exhibiting a sensitivity of 0.15  $\mu$ molL<sup>-1</sup> and detection limit of 20 nmolL<sup>-1</sup>. The MagNP/C-dots/SPE sensor was also successfully applied for the determination of NADH in serum samples. The interference of typical biological molecules has also been investigated.

**ELECTROANALYSIS 29[8], 1968-1975, 2017.** DOI: 10.1002/elan.201700167

**[P210-2017] “Measurement of D-meson production at mid-rapidity in pp collisions at  $\sqrt{s}=7$  TeV”**

Acharya, S.; Adamova, D.; Aggarwal, M. M.; Albuquerque, D. S. D.\*; Chinellato, D. D.\*; De Souza, R. D.\*; Takahashi, J.\*; et al.  
ALICE Collaboration

The production cross sections for prompt charmed mesons D<sup>0</sup>, D<sup>+</sup>, D<sup>\*+</sup> and D-s(+) were measured at mid-rapidity in proton-proton collisions at a centre-of-mass energy  $\sqrt{s} = 7$  TeV with the ALICE detector at the Large Hadron Collider (LHC). D mesons were reconstructed from their decays D<sup>0</sup> → K-pi(+), D<sup>+</sup> → K-pi(+), D<sup>\*+</sup> → D<sup>0</sup> pi(+), D-s(+) → phi pi(+), and their charge conjugates. With respect to previous measurements in the same rapidity region, the coverage in transverse momentum (p(T)) is extended and the uncertainties are reduced by a factor of about two. The accuracy on the estimated total c (c) over bar production cross section is likewise improved. The measured p(T)-differential cross sections are compared with the results of three perturbative QCD calculations.

**EUROPEAN PHYSICAL JOURNAL C 77[8], 550, 2017.** DOI: 10.1140/epjc/s10052-017-5090-4

**[P211-2017] “Measurement of double-differential cross sections for top quark pair production in pp collisions at  $\sqrt{s}=8$  TeV and impact on parton distribution functions”**

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

Normalized double-differential cross sections for top quark pair (t (t) over bar) production are measured in pp collisions at a centre-of-mass energy of 8 TeV with the CMS experiment at the LHC. The analyzed data correspond to an integrated luminosity of 19.7 fb<sup>-1</sup>. The measurement is performed in the dilepton e(+/-)mu(+/-) final state. The tt cross section is determined as a function of various pairs of observables characterizing the kinematics of the top quark and tt system. The data are compared to calculations using perturbative quantum chromodynamics at next-to-leading and approximate next-to-next-to-leading orders. They are also compared to predictions of Monte Carlo event generators that complement fixed-order computations with parton showers, hadronization, and multiple-parton interactions. Overall agreement is observed with the predictions, which is improved when the latest global sets of proton parton distribution functions are used. The inclusion of the measured tt cross sections in a fit of parametrized parton distribution functions is shown to have significant impact on the gluon distribution.

**EUROPEAN PHYSICAL JOURNAL C 77[7], 459, 2017.** DOI: 10.1140/epjc/s10052-017-4984-5

**[P212-2017] “Measurement of electrons from beauty-hadron decays in p-Pb collisions at  $\sqrt{\text{NN}}\text{-N-S}=5.02$  TeV and Pb-Pb collisions at  $\sqrt{\text{NN}}\text{-N-S}=2.76$  TeV”**

Adam, J.; Adamova, D.; Aggarwal, M. M.; Albuquerque, D. S. D.\*; Chinellato, D. D.\*; De Souza, R. D.\*; Takahashi, J.\*; et al.  
ALICE Collaboration

The production of beauty hadrons was measured via semi-leptonic decays at mid-rapidity with the ALICE detector at the LHC in the transverse momentum interval  $1 < PT < 8$  GeV/c in minimum-bias p-Pb collisions at  $\sqrt{\text{NN}}\text{-N-S} = 5.02$  TeV and in  $1.3 < PT < 8$  GeV/c in the 20% most central Pb-Pb collisions at  $\sqrt{\text{NN}}\text{-N-S} = 2.76$  TeV. The pp reference spectra at  $\sqrt{s} = 5.02$  TeV and  $\sqrt{s} = 2.76$  TeV, needed for the calculation of the nuclear modification factors R<sub>pPb</sub> and R<sub>PbPb</sub>,

were obtained by a pQCD-driven scaling of the cross section of electrons from beauty-hadron decays measured at  $\sqrt{s} = 7$  TeV. In the PT interval  $3 < PT < 8$  GeV/c, a suppression of the yield of electrons from beauty-hadron decays is observed in Pb-Pb compared to pp collisions. Towards lower PT, the R-PbPb values increase with large systematic uncertainties. The R-ppb is consistent with unity within systematic uncertainties and is well described by theoretical calculations that include cold nuclear matter effects in p-Pb collisions. The measured R-pPb and these calculations indicate that cold nuclear matter effects are small at high transverse momentum also in Pb-Pb collisions. Therefore, the observed reduction of R-PbPb below unity at high PT may be ascribed to an effect of the hot and dense medium formed in Pb-Pb collisions.

**JOURNAL OF HIGH ENERGY PHYSICS 7, 052, 2017. DOI: 10.1007/JHEP07(2017)052**

**[P213-2017] “Measurement of inclusive jet cross sections in pp and PbPb collisions at  $\sqrt{s(NN)}=2.76$  TeV”**

Khachatryan, V.; Sirunyan, A. M.; Tumasyan, A.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

Inclusive jet spectra from pp and PbPb collisions at a nucleon-nucleon center-of-mass energy of 2.76 TeV, collected with the CMS detector at the CERN Large Hadron Collider, are presented. Jets are reconstructed with three different distance parameters ( $R = 0.2, 0.3, \text{ and } 0.4$ ) for transverse momentum ( $p(T)$ ) greater than 70 GeV/c and pseudorapidity  $|\eta| < 2$ . Next-to-leading-order quantum chromodynamic calculations with nonperturbative corrections are found to overpredict jet production cross sections in pp for small distance parameters. The jet nuclear modification factors for PbPb compared to pp collisions, show a steady decrease from peripheral to central events, along with a weak dependence on the jet  $p(T)$ . They are found to be independent of the distance parameter in the measured kinematic range.

**PHYSICAL REVIEW C 96[1], 015202, 2017. DOI: 10.1103/PhysRevC.96.015202**

**[P214-2017] “Measurement of the differential inclusive B+ hadron cross sections in pp collisions at  $\sqrt{s}=13$ TeV”**

Khachatryan, V.; Sirunyan, A. M.; Tumasyan, A.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

The differential cross sections for inclusive production of B+ hadrons are measured as a function of the B+ transverse momentum  $p(T)(B)$  and rapidity  $y(B)$  in pp collisions at a centre-of-mass energy of 13 TeV, using data collected by the CMS experiment that correspond to an integrated luminosity of 48.1 pb<sup>-1</sup>. The measurement uses the exclusive decay channel  $B^+ \rightarrow J/\psi K^+$ , with J/psi mesons that decay to a pair of muons. The results show a reasonable agreement with theoretical calculations within the uncertainties.

**PHYSICS LETTERS B 771, 435-456, 2017. DOI: 10.1016/j.physletb.2017.05.074**

**[P215-2017] “Measurement of the inclusive energy spectrum in the very forward direction in proton-proton collisions at  $\sqrt{s}=13$  TeV”**

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

The differential cross section for inclusive particle production as a function of energy in proton-proton collisions at a center-of-mass energy of 13 TeV is measured in the very forward region of the CMS detector. The measurement is based on data collected with the CMS apparatus at the LHC, and corresponds to an integrated luminosity of 0.34 mu b<sup>-1</sup>. The energy is measured in the CASTOR calorimeter, which covers the pseudorapidity region  $-6.6 < \eta < -5.2$ . The results are given as a function of the total energy deposited in CASTOR, as well as of its electromagnetic and hadronic components. The spectra are sensitive to the modeling of multiparton interactions in pp collisions, and provide new constraints for hadronic interaction models used in collider and in high energy cosmic ray physics.

**JOURNAL OF HIGH ENERGY PHYSICS 8, 046, 2017. DOI: 10.1007/JHEP08(2017)046**

**[P216-2017] “Measurement of the jet mass in highly boosted t(t)over-bar events from pp collisions at  $\sqrt{s}=8$ TeV”**

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

The first measurement of the jet mass  $m(\text{jet})$  of top quark jets produced in  $t(t)$  over bar events from pp collisions at  $\sqrt{s} = 8$  TeV is reported for the jet with the largest transverse momentum  $p(T)$  in highly boosted hadronic top quark decays. The data sample, collected with the CMS detector, corresponds to an integrated luminosity of 19.7 fb<sup>-1</sup>. The measurement is performed in the lepton+jets channel in which the products of the semileptonic decay  $t \rightarrow bW$  with  $W \rightarrow l \nu$  where  $l$  is an electron or muon, are used to select  $t(t)$  over bar events with large Lorentz boosts. The products of the fully hadronic decay  $t \rightarrow bW$  with  $W \rightarrow q(q)$  over bar are reconstructed using a single Cambridge-Aachen jet with distance parameter  $R = 1.2$ , and  $pT > 400$  GeV. The  $t(t)$  over bar cross section as a function of  $m(\text{jet})$  is unfolded at the particle level and is used to test the modelling of highly boosted top quark production. The peak position of the  $m(\text{jet})$  distribution is sensitive to the top quark mass  $m(t)$ , and the data are used to extract a value of  $m(t)$  to assess this sensitivity.

**EUROPEAN PHYSICAL JOURNAL C 77[7], 467, 2017. DOI: 10.1140/epjc/s10052-017-5030-3**

**[P217-2017] “Measurement of the production of high-p(T) electrons from heavy-flavour hadron decays in Pb-Pb collisions at  $\sqrt{s(NN)}=2.76$  TeV”**

Adam, J.; Adamova, D.; Aggarwal, M. M.; Albuquerque, D. S. D.\*; Chinellato, D. D.\*; De Souza, R. D.\*; Takahashi, J.\*; et al.  
ALICE Collaboration

Electrons from heavy-flavour hadron decays (charm and beauty) were measured with the ALICE detector in Pb-Pb collisions at a centre-of-mass energy  $\sqrt{s(NN)} = 2.76$  TeV. The transverse momentum ( $pT$ ) differential production yields at mid-rapidity were used to calculate the nuclear modification factor R-AA in the interval  $3 < p(T) < 18$  GeV/c. The R-AA shows a strong suppression compared to binary scaling of pp collisions at the same energy (up to a factor of 4) in the 10% most central Pb-Pb collisions. There is a centrality trend of suppression, and a weaker suppression (down to a factor of 2) in semi-peripheral (50-80%) collisions is observed. The suppression of electrons in this broad  $p(T)$  interval indicates that both charm and beauty quarks lose energy when they traverse the hot medium formed in Pb-Pb collisions at LHC.

**PHYSICS LETTERS B 771, 467-481, 2017. DOI: 10.1016/j.physletb.2017.05.060**

**[P218-2017] “Measurement of the top quark mass in the dileptonic  $t(\bar{t})$  over-bar decay channel using the mass observables  $M_{bl}$ ,  $M_{T2}$ , and  $M_{blv}$  in pp collisions at  $\sqrt{s}=8$  TeV”**

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A measurement of the top quark mass ( $M_t$ ) in the dileptonic  $t(\bar{t})$  over bar decay channel is performed using data from proton-proton collisions at a center-of-mass energy of 8 TeV. The data was recorded by the CMS experiment at the LHC and corresponds to an integrated luminosity of  $19.7 \pm 0.5 \text{ fb}^{-1}$ . Events are selected with two oppositely charged leptons ( $l = e, \mu$ ) and two jets identified as originating from b quarks. The analysis is based on three kinematic observables whose distributions are sensitive to the value of  $M_t$ . An invariant mass observable,  $M_{bl}$ , and a “stransverse mass” observable,  $M_{T2}$ , are employed in a simultaneous fit to determine the value of  $M_t$  and an overall jet energy scale factor (JSF). A complementary approach is used to construct an invariant mass observable,  $M_{blv}$ , that is combined with  $M_{T2}$  to measure  $M_t$ . The shapes of the observables, along with their evolutions in  $M_t$  and JSF, are modeled by a nonparametric Gaussian process regression technique. The sensitivity of the observables to the value of  $M_t$  is investigated using a Fisher information density method. The top quark mass is measured to be  $172.22 \pm 0.18(\text{stat})(-0.93)(+0.89)$  (syst) GeV.

PHYSICAL REVIEW D 96[3], 032002, 2017. DOI: 10.1103/PhysRevD.96.032002

**[P219-2017] “Mechanical stability of the CMS strip tracker measured with a laser alignment system”**

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

The CMS tracker consists of  $206\text{m}^2$  of silicon strip sensors assembled on carbon fibre composite structures and is designed for operation in the temperature range from  $-25$  to  $+25$  degrees C. The mechanical stability of tracker components during physics operation was monitored with a few  $\mu\text{m}$  resolution using a dedicated laser alignment system as well as particle tracks from cosmic rays and hadron-hadron collisions. During the LHC operational period of 2011-2013 at stable temperatures, the components of the tracker were observed to experience relative movements of less than  $30 \mu\text{m}$ . In addition, temperature variations were found to cause displacements of tracker structures of about  $2 \mu\text{m}/\text{degrees C}$ , which largely revert to their initial positions when the temperature is restored to its original value.

JOURNAL OF INSTRUMENTATION 12, P04023, 2017. DOI: 10.1088/1748-0221/12/04/P04023

**[P220-2017] “Muon counting using silicon photomultipliers in the AMIGA detector of the Pierre Auger observatory”**

Aab, A.; Abreu, P.; Aglietta, M.; Chinellato, J. A.\*; Daniel, B.\*; Diaz Castro, M. L.\*; Dobrigkeit, C.\*; Escobar, C. O.\*; Fauth, A. C.\*; Kemp, E.\*; Muller, M. A.\*; Selmi-Dei, D. Pakk\*; Pereira, L. A. S.\*; Theodoro, V. M.\*; et al.  
Pierre Auger collaboration

AMIGA (Auger Muons and Infill for the Ground Array) is an upgrade of the Pierre Auger Observatory designed to extend its energy range of detection and to directly measure the muon content of the cosmic ray primary particle showers. The array will be formed by an infill of surface water-Cherenkov detectors associated with buried scintillation counters employed for muon counting. Each counter is composed of three scintillation modules, with a  $10\text{m}^2$  detection area per module.

In this paper, a new generation of detectors, replacing the current multi-pixel photomultiplier tube (PMT) with silicon photo sensors (aka. SiPMs), is proposed. The selection of the new device and its front-end electronics is explained. A method to calibrate the counting system that ensures the performance of the detector is detailed. This method has the advantage of being able to be carried out in a remote place such as the one where the detectors are deployed. High efficiency results, i.e. 98% efficiency for the highest tested overvoltage, combined with a low probability of accidental counting (similar to 2 %), show a promising performance for this new system.

JOURNAL OF INSTRUMENTATION 12, P03002, 2017. DOI: 10.1088/1748-0221/12/03/P03002

**[P221-2017] “Nanoscale deformation and friction characteristics of atomically thin WSe<sub>2</sub> and heterostructure using nanoscratch and Raman spectroscopy”**

Manimunda, P.; Nakanishi, Y.; Jaques, Y. M.\*; Susarla, S.; Woellner, C. F.\*; Bhowmick, S.; Asif, S. A. S.; Galvao, D. S.\*; Tiwary, C. S.; Ajayan, P. M.

2D transition metals di-selenides are attracting a lot of attention due to their interesting optical, chemical and electronics properties. Here, the deformation characteristics of monolayer, multi-layer WSe<sub>2</sub> and its heterostructure with MoSe<sub>2</sub> were investigated using a new technique that combines nanoscratch and Raman spectroscopy. The 2D monolayer WSe<sub>2</sub> showed anisotropy in deformation. Effect of number of WSe<sub>2</sub> layers on friction characteristics were explored in detail. Experimental observations were further supported by MD simulations. Raman spectra recorded from the scratched regions showed strain induced degeneracy splitting. Further nano-scale scratch tests were extended to MoSe<sub>2</sub>-WSe<sub>2</sub> lateral heterostructures. Effect of deformation on lateral hetero junctions were further analysed using PL and Raman spectroscopy. This new technique is completely general and can be applied to study other 2D materials.

2D MATERIALS 4[4], 045005, 2017. DOI: 10.1088/2053-1583/aa8475

**[P222-2017] “Nematic fluctuations and phase transitions in LaFeAsO: A Raman scattering study”**

Kaneko, U. F.\*; Gomes, P. F.; Garcia-Flores, A. F.; Yan, J. -Q.; Lograsso, T. A.; Barberis, G. E.\*; Vaknin, D.; Granado, E.\*

Raman scattering experiments on LaFeAsO with distinct antiferromagnetic ( $T_{AFM} = 140$  K) and tetragonal-orthorhombic ( $T_S = 155$  K) transitions show a quasielastic peak (QEP) in B-2g symmetry (2 Fe tetragonal cell) that fades away below similar to T-AFM and is ascribed to electronic nematic fluctuations. A scaling of the reported shear modulus with the T dependence of the QEP height rather than the QEP area indicates that magnetic degrees of freedom drive the structural transition. The large separation between T-S and T-AFM in LaFeAsO compared to BaFe<sub>2</sub>As<sub>2</sub> manifests itself in slower dynamics of nematic fluctuations in the former.

PHYSICAL REVIEW B 96[1], 014506, DOI: 10.1103/PhysRevB.96.014506

**[P223-2017] “Non-Abelian Ball-Chiu vertex for arbitrary Euclidean momenta”**

Aguilar, A. C.\*; Cardona, J. C.\*; Ferreira, M. N.\*; Papavassiliou, J.



We determine the non-Abelian version of the four nontransverse form factors of the quark-gluon vertex, using exact expressions derived from the Slavnov-Taylor identity that this vertex satisfies. In addition to the quark and ghost propagators, a key ingredient of the present approach is the quark-ghost scattering kernel, which is computed within the one-loop dressed approximation. The vertex form factors obtained from this procedure are evaluated for arbitrary Euclidean momenta, and display features not captured by the well-known Ball-Chiu vertex, deduced from the Abelian (ghost-free) Ward identity. Particularly interesting in this analysis is the so-called soft-gluon limit, which, unlike other kinematic configurations considered, is especially sensitive to the approximations employed for the vertex entering in the quark-ghost scattering kernel, and may even be affected by a subtle numerical instability. As an elementary application of the results obtained, we evaluate and compare certain renormalization-point-independent combinations, which contribute to the interaction kernels appearing in the standard quark gap and Bethe-Salpeter equations. In doing so, even though all form factors of the quark-gluon vertex, and in particular the transverse ones which are unconstrained by our procedure, enter nontrivially in the aforementioned kernels, only the contribution of a single form factor, corresponding to the classical (tree-level) tensor, will be considered.

PHYSICAL REVIEW D 96[1], 014029, DOI: 10.1103/PhysRevD.96.014029

**[P224-2017] “Noninvasive optical monitoring of critical closing pressure and arteriole compliance in human subjects”**

Baker, W. B.; Parthasarathy, A. B.; Gannon, K. P.; Kavuri, V. C.; Busch, D. R.; Abramson, K.; He, L.; Mesquita, R. C.\*; Mullen, M. T.; Detre, J. A.; Greenberg, J. H.; Licht, D. J.; Balu, R.; Kofke, W. A.; Yodh, A. G.

The critical closing pressure (CrCP) of the cerebral circulation depends on both tissue intracranial pressure and vasomotor tone. CrCP defines the arterial blood pressure (ABP) at which cerebral blood flow approaches zero, and their difference (ABP - CrCP) is an accurate estimate of cerebral perfusion pressure. Here we demonstrate a novel noninvasive technique for continuous monitoring of CrCP at the bedside. The methodology combines optical diffuse correlation spectroscopy (DCS) measurements of pulsatile cerebral blood flow in arterioles with concurrent ABP data during the cardiac cycle. Together, the two waveforms permit calculation of CrCP via the two-compartment Windkessel model for flow in the cerebral arterioles. Measurements of CrCP by optics (DCS) and transcranial Doppler ultrasound (TCD) were carried out in 18 healthy adults; they demonstrated good agreement ( $R = 0.66$ , slope =  $1.14 \pm 0.23$ ) with means of  $11.1 \pm 5.0$  and  $13.0 \pm 7.5$  mmHg, respectively. Additionally, a potentially useful and rarely measured arteriole compliance parameter was derived from the phase difference between ABP and DCS arteriole blood flow waveforms. The measurements provide evidence that DCS signals originate predominantly from arteriole blood flow and are well suited for long-term continuous monitoring of CrCP and assessment of arteriole compliance in the clinic.

JOURNAL OF CEREBRAL BLOOD FLOW AND METABOLISM 37[8], 2691-2705, 2017. DOI: 10.1177/0271678X17709166

**[P225-2017] “Optimizing Weak Measurements to Detect Angular Deviations”**

Araujo, M. P.\*; De Leo, S.; Maia, G. G.\*

We analyze and compare the angular deviations for an optical beam reflected by and transmitted through a dielectric triangular prism. The analytic expressions derived for the angular deviations hold for arbitrary incidence angles.

For incidence approaching the internal and external Brewster angles, the angular deviations transverse magnetic waves present the same behavior leading to the well-known giant Goos-Hanchen angular shift. For incidence near the critical angle a new region of large shift is seen both for transverse magnetic and transverse electric waves. While a direct measuring procedure is better in the vicinity of the Brewster region, a weak measurement breaks off the giant Goos-Hanchen effect, preserving the amplification in the critical region. We discuss under which conditions it is possible to optimize the amplification and we also determine when a weak measurement is preferred to a direct measuring procedure.

ANNALEN DER PHYSIK 529[9], 1600357, 2017. DOI: 10.1002/andp.201600357

**[P226-2017] “Probing atmospheric mixing and leptonic CP violation in current and future long baseline oscillation experiments”**

Chatterjee, S. S.; Pasquini, P.\*; Vane, J. W. F.

We perform realistic simulations of the current and future long baseline experiments such as T2K, NOvA, DUNE and T2HK in order to determine their ultimate potential in probing neutrino oscillation parameters. We quantify the potential of these experiments to underpin the octant of the atmospheric angle  $\theta_{23}$  as well as the value and sign of the CP phase  $\delta_{CP}$ . We do this both in general, as well as within the predictive framework of a previously proposed [1] benchmark theory of neutrino oscillations which tightly correlates  $\theta_{23}$  and  $\delta_{CP}$ .

PHYSICS LETTERS B 771, 524-531, 2017. DOI: 10.1016/j.physletb.2017.05.080

**[P227-2017] “Protonic charge defect structures in floating water bridges observed as Zundel and Eigen solvation arrangements”**

Teschke, O.\*; de Castro, J. R.\*; Valente Filho, J. F.\*; Soares, D. M.\*

Protonic arrangements were detected in water bridge structures using confocal Raman microscopy, and the spectra show two formed structures. The measured Raman spectra were modified using the voltage applied to the bridge structure, which changed the proportion of these two species. Initially, for a 6.3 kV applied voltage, there was a measurable increase in the bridge current above the Ohmic contribution and the observed Raman spectrum of this new injected specie corresponded to the computed spectrum for the Zundel protonic arrangement. As the voltage further increases a contribution from the Eigen proton solvation specie is added to the measured spectrum.

CHEMICAL PHYSICS LETTERS 685, 239-243, 2017. DOI: 10.1016/j.cplett.2017.07.063

**[P228-2017] “Pseudorapidity dependence of long-range two-particle correlations in pPb collisions at root sNN=5.02 TeV”**

Khachatryan, V.; Sirunyan, A. M.; Tumasyan, A.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

Two-particle correlations in pPb collisions at a nucleon-nucleon center-of-mass energy of 5.02 TeV are studied as a function of the pseudorapidity separation ( $\Delta\eta$ ) of the particle pair at small relative azimuthal angle ( $|\Delta\phi| < \pi/3$ ). The correlations are decomposed into a jet component that dominates the short-range correlations ( $|\Delta\eta| < 1$ ),

and a component that persists at large Delta eta and may originate from collective behavior of the produced system. The events are classified in terms of the multiplicity of the produced particles. Finite azimuthal anisotropies are observed in high-multiplicity events. The second and third Fourier components of the particle-pair azimuthal correlations,  $V_2$  and  $V_3$ , are extracted after subtraction of the jet component. The single-particle anisotropy parameters  $v_2$  and  $v_3$  are normalized by their laboratory frame midrapidity value and are studied as a function of  $\eta(\text{c.m.})$ . The normalized  $v_2$  distribution is found to be asymmetric about  $\eta(\text{c.m.}) = 0$ , with smaller values observed at forward pseudorapidity, corresponding to the direction of the proton beam, while no significant pseudorapidity dependence is observed for the normalized  $v_3$  distribution within the statistical uncertainties.

PHYSICAL REVIEW C 96[1], 014915, 2017. DOI: 10.1103/PhysRevC.96.014915

[P229-2017] “Quantum scattering on a cone revisited”

Barroso, V. S.\*; Pitelli, J. P. M.

We revisit the scattering of quantum test particles on the conical  $(2 + 1)$ -dimensional spacetime and find the scattering amplitude as a function of the boundary conditions imposed at the apex of the cone. We show that the boundary condition is responsible for a purely analytical term in the scattering amplitude, in addition to those coming from purely topological effects. Since it is possible to have nonequivalent physical evolutions for the wave packet (each one corresponding to a different boundary condition), it seems crucial to have an observable quantity specifying which evolution has been prescribed.

PHYSICAL REVIEW D 96[2], 025006, 2017. DOI: 10.1103/PhysRevD.96.025006

[P210-2017] “Range Extension in Coherent OFDM Passive Optical Networks Using an Inverse Hammerstein Nonlinear Equalizer”

Torres-Zugaide, J.; Aldaya, I.\*; Campuzano, G.; Giacomidis, E.; Beas, J.; Castanon, G.

High-speed demand driven by bandwidth-consuming applications, such as video streaming and cloud computing, is exceeding available network capacity, forcing operators to implement innovative technologies to increase the throughput offered to end users. In particular, passive optical networks (PONs) with a full-duplex capacity of 10 Gb/s over a 40-km span are expected to be developed shortly. However, the range of such systems is severely penalized due to fiber and splitter losses. To increase the transmission distance of PONs, coherent optical (CO) communications have regained attention. Orthogonal frequency division multiplexing (OFDM) has been proposed as a modulation format due to its robustness to chromatic dispersion, high spectral efficiency, and flexibility. The high peak-to-average ratio of OFDM signals, however, makes them very vulnerable to fiber nonlinear distortion. In this paper, we propose what we believe is a novel, low-complexity equalizer based on the inverse Hammerstein model to partially compensate for the nonlinear distortion in CO-OFDM PONs. Numerical simulations using the split-step Fourier transform method reveal a potential link increase of 20 and 5 km for bit rates of 10 and 40 Gb/s, respectively, when compared to linear equalization.

JOURNAL OF OPTICAL COMMUNICATIONS AND NETWORKING 9[7], 577-584, 2017. DOI: 10.1364/JOCN.9.000577

[P211-2017] “Resolving the atmospheric octant by an improved measurement of the reactor angle”

Chatterjee, S. S.; Pasquini, P.\*; Valle, J. W. F.

Taking into account the current global information on neutrino oscillation parameters we forecast the capabilities of future long-baseline experiments such as DUNE and T2HK in settling the atmospheric octant puzzle. We find that a good measurement of the reactor angle  $\theta_{13}$  plays a key role in fixing the octant of the atmospheric angle  $\theta_{23}$  with such future accelerator neutrino studies.

PHYSICAL REVIEW D 96[1], 011303, 2017. DOI: 10.1103/PhysRevD.96.011303

[P212-2017] “Search for associated production of a Z boson with a single top quark and for  $tZ$  flavour-changing interactions in pp collisions at  $\sqrt{s}=8$  TeV”

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A search for the production of a single top quark in association with a Z boson is presented, both to identify the expected standard model process and to search for flavour changing neutral current interactions. The data sample corresponds to an integrated luminosity of 19.7 fb<sup>-1</sup> recorded by the CMS experiment at the LHC in proton-proton collisions at  $\sqrt{s} = 8$  TeV. Final states with three leptons (electrons or muons) and at least one jet are investigated. An events yield compatible with  $tZ$  standard model production is observed, and the corresponding cross section is measured to be  $\sigma(\text{pp} \rightarrow tZ \rightarrow \text{lvbl}(+)\text{l}(-)q) = 10(-7)(+8)$  fb with a significance of 2.4 standard deviations. No presence of flavour-changing neutral current production of  $tZ$  is observed. Exclusion limits at 95% confidence level on the branching fractions of a top quark decaying to a Z boson and an up or a charm quark are found to be  $\text{B}(t \rightarrow Z\text{u}) < 0.022\%$  and  $\text{B}(t \rightarrow Z\text{c}) < 0.049\%$ .

JOURNAL OF HIGH ENERGY PHYSICS 7, 003, 2017. DOI: 10.1007/JHEP07(2017)003

[P213-2017] “Search for dark matter produced with an energetic jet or a hadronically decaying W or Z boson at  $\sqrt{S}=13$  TeV”

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A search for dark matter particles is performed using events with large missing transverse momentum, at least one energetic jet, and no leptons, in proton-proton collisions at  $\sqrt{S} = 13\text{TeV}$  collected with the CMS detector at the LHC. The data sample corresponds to an integrated luminosity of 12.9 fb<sup>-1</sup>. The search includes events with jets from the hadronic decays of a W or Z boson. The data are found to be in agreement with the predicted background contributions from standard model processes. The results are presented in terms of simplified models in which dark matter particles are produced through interactions involving a vector, axial-vector, scalar, or pseudoscalar mediator. Vector and axial-vector mediator particles with masses up to 1.95TeV, and scalar and pseudoscalar mediator particles with masses up to 100 and 430 GeV respectively, are excluded at 95% confidence level. The results are also interpreted in terms of the invisible decays of the Higgs boson, yielding an observed (expected) 95% confidence level upper limit of 0.44 (0.56) on the corresponding branching fraction. The results of this search provide the strongest constraints on the dark matter pair production cross section through vector and axial-vector mediators at a particle collider. When compared to the direct detection experiments, the limits obtained from this search provide stronger

constraints for dark matter masses less than 5, 9, and 550 GeV, assuming vector, scalar, and axial-vector mediators, respectively. The search yields stronger constraints for dark matter masses less than 200 GeV, assuming a pseudoscalar mediator, when compared to the indirect detection results from Fermi-LAT.

**JOURNAL OF HIGH ENERGY PHYSICS 7, 014, 2017. DOI: 10.1007/JHEP07(2017)014**

**[P214-2017] “Search for new physics with dijet angular distributions in proton-proton collisions at root S = 13 TeV”**

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A search is presented for extra spatial dimensions, quantum black holes, and quark contact interactions in measurements of dijet angular distributions in proton-proton collisions at root S = 13TeV. The data were collected with the CMS detector at the LHC and correspond to an integrated luminosity of 2.6 fb(-1). The distributions are found to be in agreement with predictions from perturbative quantum chromodynamics that include electroweak corrections. Limits for different contact interaction models are obtained. In a benchmark model, valid to next-to-leading order in QCD and in which only left-handed quarks participate, quark contact interactions are excluded up to a scale of 11.5 and 14.7TeV for destructive or constructive interference, respectively. The production of quantum black holes is excluded for masses below 7.8 or 5.3TeV, depending on the model. The lower limits for the scales of virtual graviton exchange in the Arkani-HamedDimopoulos-Dvali model of extra spatial dimensions are in the range 7.9-11.2TeV, and are the most stringent set of limits available.

**JOURNAL OF HIGH ENERGY PHYSICS 7, 013, 2017. DOI: 10.1007/JHEP07(2017)013**

**[P215-2017] “Search for physics beyond the standard model in events with two leptons of same sign, missing transverse momentum, and jets in proton-proton collisions at root s=13TeV”**

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A data sample of events from proton-proton collisions with two isolated same-sign leptons, missing transverse momentum, and jets is studied in a search for signatures of new physics phenomena by the CMS Collaboration at the LHC. The data correspond to an integrated luminosity of 35.9 fb(-1), and a center-of-mass energy of 13 TeV. The properties of the events are consistent with expectations from standard model processes, and no excess yield is observed. Exclusion limits at 95% confidence level are set on cross sections for the pair production of gluinos, squarks, and same-sign top quarks, as well as top-quark associated production of a heavy scalar or pseudoscalar boson decaying to top quarks, and on the standard model production of events with four top quarks. The observed lower mass limits are as high as 1500 GeV for gluinos, 830 GeV for bottom squarks. The excluded mass range for heavy (pseudo) scalar bosons is 350-360 (350-410) GeV. Additionally, model-independent limits in several topological regions are provided, allowing for further interpretations of the results.

**EUROPEAN PHYSICAL JOURNAL C 77[9], 578, 2017. DOI: 10.1140/epjc/s10052-017-5079-z**

**[P216-2017] “Search for single production of a heavy vector-like T quark decaying to a Higgs boson and a top quark with a lepton and jets in the final state”**

Khachatryan, V.; Sirunyan, A. M.; Tumasyan, A.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A search for single production of vector-like top quark partners (T) decaying into a Higgs boson and a top quark is performed using data from pp collisions at a center-of-mass energy of 13 TeV collected by the CMS experiment at the CERN LHC, corresponding to an integrated luminosity of 2.3 fb(-1). The top quark decay includes an electron or a muon while the Higgs boson decays into a pair of b quarks. No significant excess over standard model backgrounds is observed. Exclusion limits on the product of the production cross section and the branching fraction are derived in the T quark mass range 700 to 1800 GeV. For a mass of 1000 GeV, values of the product of the production cross section and the branching fraction greater than 0.8 and 0.7 pb are excluded at 95% confidence level, assuming left- and right-handed coupling of the T quark to standard model particles, respectively. This is the first analysis setting exclusion limits on the cross section of singly produced vector-like T quarks at a center-of-mass energy of 13 TeV.

**PHYSICS LETTERS B 771, 80-105, 2017. DOI: 10.1016/j.physletb.2017.05.019**

**[P217-2017] “Search for supersymmetry in multijet events with missing transverse momentum in proton-proton collisions at 13 TeV”**

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A search for supersymmetry is presented based on multijet events with large missing transverse momentum produced in proton-proton collisions at a center-of-mass energy of root s = 13 TeV. The data, corresponding to an integrated luminosity of 35.9 fb(-1), were collected with the CMS detector at the CERN LHC in 2016. The analysis utilizes four-dimensional exclusive search regions defined in terms of the number of jets, the number of tagged bottom quark jets, the scalar sum of jet transverse momenta, and the magnitude of the vector sum of jet transverse momenta. No evidence for a significant excess of events is observed relative to the expectation from the standard model. Limits on the cross sections for the pair production of gluinos and squarks are derived in the context of simplified models. Assuming the lightest supersymmetric particle to be a weakly interacting neutralino, 95% confidence level lower limits on the gluino mass as large as 1800 to 1960 GeV are derived, and on the squark mass as large as 960 to 1390 GeV, depending on the production and decay scenario.

**PHYSICAL REVIEW D 96[3], 032003, 2017. DOI: 10.1103/PhysRevD.96.032003**

**[P218-2017] “Search for supersymmetry in the all-hadronic final state using top quark tagging in pp collisions at root s=13 TeV”**

Khachatryan, V.; Sirunyan, A. M.; Tumasyan, A.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A search is presented for supersymmetry in all-hadronic events with missing transverse momentum and tagged top quarks. The data sample was collected with the CMS detector at the LHC and corresponds to an integrated luminosity of 2.3 fb(-1) of proton-proton collisions at a center-of-mass energy of 13 TeV. Search regions are defined using the properties of reconstructed jets, the multiplicity of bottom and top quark candidates, and an imbalance in transverse momentum. With no statistically significant excess of events observed beyond the expected contributions from the standard model,



we set exclusion limits at 95% confidence level on the masses of new particles in the context of simplified models of direct and gluino-mediated top squark production. For direct top squark production with decays to a top quark and a neutralino, top squark masses up to 740 GeV and neutralino masses up to 240 GeV are excluded. Gluino masses up to 1550 GeV and neutralino masses up to 900 GeV are excluded for a gluino-mediated production case, where each of the pair-produced gluinos decays to a top-antitop quark pair and a neutralino.

PHYSICAL REVIEW D 96[1], 012004, 2017. DOI: 10.1103/PhysRevD.96.012004

[P219-2017] “Search for third-generation scalar leptoquarks and heavy right-handed neutrinos in final states with two tau leptons and two jets in proton-proton collisions at root  $s=13$  TeV”

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A search is performed for third-generation scalar leptoquarks and heavy right-handed neutrinos in events containing one electron or muon, one hadronically decaying tau lepton, and at least two jets, using a root  $s = 13$  TeV pp collision data sample corresponding to an integrated luminosity of 12: 9 fb(-1) collected with the CMS detector at the LHC in 2016. The number of observed events is found to be in agreement with the standard model prediction. A limit is set at 95% confidence level on the product of the leptoquark pair production cross section and  $\beta(2)$ , where  $\beta$  is the branching fraction of leptoquark decay to a tau lepton and a bottom quark. Assuming  $\beta = 1$ , third-generation leptoquarks with masses below 850 GeV are excluded at 95% confidence level. An additional search based on the same event topology involves heavy right-handed neutrinos, N-R, and right-handed W bosons, W-R, arising in a left-right symmetric extension of the standard model. In this search, W-R bosons are assumed to decay to a tau lepton and N-R followed by the decay of the N-R to a tau lepton and an off-shell W-R boson. Assuming the mass of the right-handed neutrino to be half of the mass of the right-handed W boson, W-R boson masses below 2.9 TeV are excluded at 95% confidence level. These results improve on the limits from previous searches for third-generation leptoquarks and heavy right-handed neutrinos with tau leptons in the final state.

JOURNAL OF HIGH ENERGY PHYSICS 7, 121, 2017. DOI: 10.1007/JHEP07(2017)121

[P220-2017] “Search for top quark partners with charge 5/3 in proton-proton collisions at root  $s=13$  TeV”

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

A search for the production of heavy partners of the top quark with charge 5/3 ( $X=5/3$ ) decaying into a top quark and a W boson is performed with a data sample corresponding to an integrated luminosity of 2.3 fb(-1), collected in proton-proton collisions at a center-of-mass energy of 13 TeV with the CMS detector at the CERN LHC. Final states with either a pair of same-sign leptons or a single lepton, along with jets, are considered. No significant excess is observed in the data above the expected standard model background contribution and an X-5/3 quark with right-handed (left-handed) couplings is excluded at 95% confidence level for masses below 1020 (990) GeV. These are the first limits based on a combination of the same-sign dilepton and the single-lepton final states, as well as the most stringent limits on the X-5/3 mass to date.

JOURNAL OF HIGH ENERGY PHYSICS 8, 073, 2017. DOI: 10.1007/JHEP08(2017)073

[P221-2017] “Searches for W ‘ bosons decaying to a top quark and a bottom quark in proton-proton collisions at 13TeV”

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

Searches are presented for heavy gauge bosons decaying into a top and a bottom quark in data collected by the CMS experiment at root  $s = 13$ TeV that correspond to an integrated luminosity of 2.2 and 2.6 fb<sup>-1</sup> in the leptonic and hadronic analyses, respectively. Two final states are analyzed, one containing a single electron, or muon, and missing transverse momentum, and the other containing multiple jets and no electrons or muons. No evidence is found for a right-handed W' boson (W'(R)) and the combined analyses exclude at 95% confidence level W'(R) with masses below 2.4TeV if  $M-W'R \gg M-vR$  (mass of the right-handed neutrino), and below 2.6TeV if  $M-W'R < M-vR$ . The results provide the most stringent limits for right-handed W' bosons in the top and bottom quark decay channel.

JOURNAL OF HIGH ENERGY PHYSICS 8[1-42], 029, 2017. DOI: 10.1007/JHEP08(2017)029

[P222-2017] “Strong-disorder approach for the Anderson localization transition”

Mard, H. J.; Hoyos, J. A.; Miranda, E.\*; Dobrosavljevic, V.

We propose a strong-disorder renormalization-group approach to study the Anderson localization transition in disordered tight-binding models in any dimension. Our approach shifts the focus from the lower to the upper critical dimension, thus emphasizing the strong-coupling/strong-disorder nature of the transition. By studying the two-point conductance, we (i) show that our approach is in excellent agreement with exact numerical results, (ii) confirm that the upper critical dimension for the Anderson transition is  $d(c)(+) = \infty$ , (iii) find that the scaling function shows a previously reported ‘mirror symmetry’ in the critical region, and (iv) demonstrate that the range of conductances for which this symmetry holds increases with the system dimensionality. Our results open an efficient avenue to explore the critical properties of the Anderson transition using the strong-coupling high-dimension limit as a starting point.

PHYSICAL REVIEW B 96[4], 045143, 2017. DOI: 10.1103/PhysRevB.96.045143

[P223-2017]“Structural and magnetic analysis of La<sub>0.67</sub>Ca<sub>0.33</sub>MnO<sub>3</sub> nanoparticles thermally treated: Acoustic detection of the magnetocaloric effect”

Pena, C. F.; Soffner, M. E.; Mansanares, A. M.\*; Sampaio, J. A.; Gandra, F. C. G.\*; da Silva, E. C.; Vargas, H.

Nanoparticles of La<sub>0.67</sub>Ca<sub>0.33</sub>MnO<sub>3</sub> were synthesized via the sol-gel method, thermally treated and characterized using X-ray diffraction, magnetization, electron spin resonance and magnetoacoustic experiments. The formation of the desired perovskite structure was verified and the average size of the nanoparticles was also determined. An increase of the particle size by rising the treatment temperature was observed. The Curie temperature and the isothermal entropy variation of the samples were obtained from the magnetization data. The isothermal entropy change, produced under the application of an external magnetic field,

which expresses the magnetocaloric effect, became significantly larger for the samples treated at higher temperatures. These results are in good agreement with those obtained by magnetoacoustics, based on the direct and contactless measurement of the temperature change, validating the ability of the technique to study the magnetocaloric effect in reduced mass and nanoparticles samples.

**PHYSICA B-CONDENSED MATTER 523, 39-44, 2017. DOI: 10.1016/j.physb.2017.08.022**

**[P224-2017] “Study of Jet Quenching with Z plus jet Correlations in Pb-Pb and pp Collisions at root s(NN)=5.02 TeV”**

Sirunyan, A. M.; Tumasyan, A.; Adam, W.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

The production of jets in association with Z bosons, reconstructed via the  $\mu^{+}\mu^{-}$  and  $e^{+}e^{-}$  decay channels, is studied in pp and, for the first time, in Pb-Pb collisions. Both data samples were collected by the CMS experiment at the LHC, at a nucleon-nucleon center-of-mass energy of 5.02 TeV. The Pb-Pb collisions were analyzed in the 0%-30% centrality range. The back-to-back azimuthal alignment was studied in both pp and Pb-Pb collisions for Z bosons with transverse momentum  $p(T)(Z) > 60$  GeV/c and a recoiling jet with  $p(T)(jet) > 30$  GeV/c. The p(T) imbalance  $x(jZ) = p(T)(jet)/p(T)(Z)$ , as well as the average number of jet partners per Z,  $R-jZ$ , was studied in intervals of  $p(T)(Z)$ . The  $R-jZ$  is found to be smaller in Pb-Pb than in pp collisions, which suggests that in Pb-Pb collisions a larger fraction of partons associated with the Z bosons fall below the 30 GeV/c  $p(T)(jet)$  threshold because they lose energy.

**PHYSICAL REVIEW LETTERS 119[8], 082301, 2017. DOI: 10.1103/PhysRevLett.119.082301**

**[P225-2017] “Super-resolution imaging of synaptic and Extra-synaptic AMPA receptors with different-sized fluorescent probes”**

Lee, S. H.; Jin, C.; Cai, E.; Ge, P.; Ishitsuka, Y.; Teng, K. W.; de Thomaz, A. A.\*; Nall, D.; Baday, M.; Jeyifous, O.; Demonte, D.; Dundas, C. M.; Park, S.; Delgado, J. Y.; Green, W. N.; Selvin, P. R.

Previous studies tracking AMPA receptor (AMPA) diffusion at synapses observed a large mobile extrasynaptic AMPAR pool. Using super-resolution microscopy, we examined how fluorophore size and photostability affected AMPAR trafficking outside of, and within, post-synaptic densities (PSDs) from rats. Organic fluorescent dyes ( $> 4$  nm), quantum dots, either small ( $> 10$  nm diameter; sQDs) or big ( $> 20$  nm; bQDs), were coupled to AMPARs via different-sized linkers. We find that  $> 90\%$  of AMPARs labeled with fluorescent dyes or sQDs were diffusing in confined nanodomains in PSDs, which were stable for 15 min or longer. Less than 10% of sQD-AMPA were extrasynaptic and highly mobile. In contrast, 5-10% of bQD-AMPA were in PSDs and 90-95% were extrasynaptic as previously observed. Contrary to the hypothesis that AMPAR entry is limited by the occupancy of open PSD ‘slots’, our findings suggest that AMPARs rapidly enter stable nanodomains in PSDs with lifetime  $> 15$  min, and do not accumulate in extrasynaptic membranes.

**ELIFE 6, e27744, 2017. DOI: 10.7554/eLife.27744**

**[P226-2017] “TDDFT-Based Study on the Proton-DNA Collision”**

Seraide, R.\*; Bernal, M. A.\*; Brunetto, G.\*; de Giovannini, U.; Rubio, A.

The interaction of heavy charged particles with DNA is of interest for hadrontherapy and the aerospace industry. Here, a time-dependent density functional theory study on the interaction of a 4 keV proton with an isolated DNA base pair (bp) was carried out. Ehrenfest dynamics was used to study the evolution of the system up to about 193 fs. It was observed that the dissociation of the target occurs between 80 and 100 fs. The effect of bp linking to the DNA double helix was emulated by fixing the four O3' atoms responsible for the attachment. The bp tends to dissociate into its main components, namely, the phosphate groups, sugars, and nitrogenous bases. A central impact with an energy transfer of 17.9 eV only produces a base damage while keeping the backbone intact. An impact on a phosphate group with an energy transfer of about 60 eV leads to a backbone break at that site together with a base damage, and the opposite backbone site integrity is kept. As the whole system is perturbed during this collision, no atom remains passive. These results suggest that base damage accompanies all backbone breaks as the hydrogen bonds that keep bases together are much weaker than those between the other components of the DNA.

**JOURNAL OF PHYSICAL CHEMISTRY B 121[30], 7276-7283, 2017. DOI: 10.1021/acs.jpcc.7b04934**

**[P227-2017] “The Effect of Stress in the Density of States of Amorphous Carbon Films Determined by X-Ray Excited Auger Electron Spectroscopy”**

Barbieri, P. F.\*; Marques, F. C.\*

Amorphous carbon films can be prepared with a large variety of structure and have been used in a number of technological applications. Many of their properties have been determined, but very little is known concerning the effect of pressure on their properties. In this work we investigate the influence of pressure of graphite-like amorphous carbon films on the density of states (DOS) using X-ray Excited Auger Electron Spectroscopy (XAES) and the second derivative method of the XAES. The films were deposited by ion beam deposition and simultaneously bombarded with argon, which is responsible for the variation of the film stress, reaching extremely high values (4.5 GPa). Marked variations of the density of states of the P-pi, P-sigma, sp, and s components were observed with increasing stress.

**ADVANCES IN MATERIALS SCIENCE AND ENGINEERING, 5826527, 2017. DOI: 10.1155/2017/5826527**

**[P228-2017] “The role of short-range magnetic correlations in the gap opening of topological Kondo insulators”**

Ramos, E.; Franco, R.; Silva-Valencia, J.; Foglio, M. E.\*; Figueira, M. S.

In this article we investigate the effects of short-range anti-ferromagnetic correlations on the gap opening of topological Kondo insulators. We add a Heisenberg term to the periodic Anderson model at the limit of strong correlations in order to allow a small degree of hopping of the localized electrons between neighboring sites of the lattice. This new model is adequate for studying topological Kondo insulators, whose paradigmatic material is the compound SmB6. The main finding of the article is that the short-range antiferromagnetic correlations, present in some Kondo insulators, contribute decisively to the opening of the Kondo gap in their density of states. These correlations are produced by the interaction between moments on the neighboring sites of the lattice. For simplicity, we solve the problem on a two dimensional square lattice. The starting point of the model is the 4f - Ce ions orbitals, with  $J = 5/2$  multiplet in the presence of spin-orbit coupling. We present results for the Kondo and for the antiferromagnetic correlation functions. We calculate the phase diagram of the model, and as we vary the E-f level position from the empty regime to the Kondo regime,

the system develops metallic and topological Kondo insulator phases. The band structure calculated shows that the model describes a strong topological insulator.

**JOURNAL OF PHYSICS-CONDENSED MATTER 29[34], 345601, 2017. DOI: 10.1088/1361-648X/aa791b**

**[P229-2017] “The role of the electrode configuration on the electrical properties of small-molecule semiconductor thin-films”**

**Merces, L.\*; de Oliveira, R. F.; Gomes, H. L.; Bufon, C. C. B.\***

This paper presents a systematic analysis of the electrode configuration influence on the electrical properties of organic semiconductor (OSC) thin-film devices. We have fabricated and electrically characterized a set of planar two-terminal devices. The differences in I-V characteristics between the top and bottom contact structures are presented and analyzed. Top-contact configurations have a linear current vs. electric field behavior, while the bottom-electrode devices display a transition from ohmic to spacecharge-limited conduction regime. The transition is temperature- and thickness-dependent. Finite-element calculations show that when the OSC film is connected using top electrodes, the current flows through the OSC bulk region. On the other hand, the bottom-electrode configuration allows most of the current to flow near the OSC/substrate interface. The current probes interfacial states resulting in a space-charge conduction regime. The results shed some light on the so-called “contact effects” commonly observed in organic thin-film transistors. The findings presented here have implications for both the understanding of the charge transport in OSC films and the design of organic semiconductor devices.

**ORGANIC ELECTRONICS 49, 107-113, 2017. DOI: 10.1016/j.orgel.2017.06.041**

**[P230-2017] “Thermodynamic DFT analysis of natural gas”**

**Neto, A. F. G.; Huda, M. N.; Marques, F. C.\*; Borges, R. S.; Neto, A. M. J. C.**

Density functional theory was performed for thermodynamic predictions on natural gas, whose B3LYP/6-311++G(d,p), B3LYP/6-31+G(d), CBS-QB3, G3, and G4 methods were applied. Additionally, we carried out thermodynamic predictions using G3/G4 averaged. The calculations were performed for each major component of seven kinds of natural gas and to their respective air + natural gas mixtures at a thermal equilibrium between room temperature and the initial temperature of a combustion chamber during the injection stage. The following thermodynamic properties were obtained: internal energy, enthalpy, Gibbs free energy and entropy, which enabled us to investigate the thermal resistance of fuels. Also, we estimated an important parameter, namely, the specific heat ratio of each natural gas; this allowed us to compare the results with the empirical functions of these parameters, where the B3LYP/6-311++G(d,p) and G3/G4 methods showed better agreements. In addition, relevant information on the thermal and mechanic resistance of natural gases were investigated, as well as the standard thermodynamic properties for the combustion of natural gas. Thus, we show that density functional theory can be useful for predicting the thermodynamic properties of natural gas, enabling the production of more efficient compositions for the investigated fuels.

**JOURNAL OF MOLECULAR MODELING 23[8], 224, 2017. DOI: 10.1007/s00894-017-3401-1**

**[P231-2017] “Two-photon absorption in a series of 2,6-disubstituted BODIPY dyes”**

**Barros, L. W. T.\*; Cardoso, T. A. S.\*; Bihlmeier, A.; Wagner, D.; Koelmel, D. K.; Hoerner, A.; Braese, S.; Cruz, C. H. B.\*; Padilha, L. A.\***

We report on the two-photon absorption spectra of a series of 2,6-disubstituted BODIPY dyes. Depending on the substituents, we observe increasing two-photon absorption cross sections with values up to 350 GM compared to 70 GM in the unsubstituted dye. Quantum chemical calculations are performed to assign the absorption bands and to understand the factors controlling the size of the two-photon absorption cross section. Both the maximum of the two-photon absorption band as well as the red-shift of the whole spectrum correlate with the ability of the substituents to extend the pi-electron system of the dye. The above-mentioned intense two-photon absorption band corresponds to the absorption of photons with 1.3 eV, which is at the first near-infrared transparency window for biological tissues. The dyes could thus be suitable for bio-imaging applications.

**PHYSICAL CHEMISTRY CHEMICAL PHYSICS 19[32], 21683-21690, 2017. DOI: 10.1039/c6cp07849d**

**[P232-2017] “Uhlenbeck-Ford model: Phase diagram and corresponding-states analysis”**

**Leite, R. P.\*; Santos-Florez, P. A.\*; de Koning, M.\***

Using molecular dynamics simulations and nonequilibrium thermodynamic-integration techniques we compute the Helmholtz free energies of the body-centered-cubic (bcc), face-centered-cubic (fcc), hexagonal close-packed, and fluid phases of the Uhlenbeck-Ford model (UFM) and use the results to construct its phase diagram. The pair interaction associated with the UFM is characterized by an ultrasoft, purely repulsive pair potential that diverges logarithmically at the origin. We find that the bcc and fcc are the only thermodynamically stable crystalline phases in the phase diagram. Furthermore, we report the existence of two reentrant transition sequences as a function of the number density, one featuring a fluid-bcc-fluid succession and another displaying a bcc-fcc-bcc sequence near the triple point. We find strong resemblances to the phase behavior of other soft, purely repulsive systems such as the Gaussian-core model (GCM), inverse-power-law, and Yukawa potentials. In particular, we find that the fcc-bcc-fluid triple point and the phase boundaries in its vicinity are in good agreement with the prediction supplied by a recently proposed corresponding-states principle [J. Chem. Phys. 134, 241101 (2011); Europhys. Lett. 100, 66004 (2012)]. The particularly strong resemblance between the behavior of the UFM and GCM models are also discussed.

**PHYSICAL REVIEW E 96[3], 032115, 2017. DOI: 10.1103/PhysRevE.96.032115**

**[P233-2017] “Unprecedented mechanical response of the lattice thermal conductivity of auxetic carbon crystals”**

**Han, Y.; Zhou, Y.; Qin, G.; Dong, J.; Galvao, D. S.\*; Hu, M.**

Lattice thermal conductivity ( $\kappa$ ) of bulk materials usually increases under compression and decreases under tension, while there are still some unusual systems, exhibiting reduced  $\kappa$  when compressed. However, to date it has never been reported for a bulk material, whose  $\kappa$  is substantially enhanced under tensile strain. In this paper, we have studied thermal transport of three auxetic carbon crystals: cis-C, trans-C and hin-C for short, and their strain responses by performing first-principles calculations. It is intriguing to find that their  $\kappa$  are much lower than those of their allotropes,



and further decrease abnormally under compression. More strikingly,  $\kappa$  of trans-C (cis-C) anomalously increases with tensile strain up to 7% (6%) with maximum  $\kappa$  of almost 7 (5) times larger than the unstrained value. The abnormal strain dependent  $\kappa$  are attributed to the dominant role of the enhancement of phonon lifetime under stretching, which can be further explained from the unique atomic structure of the main chain of polydiacetylene in trans-C and cis-C. The weakening of phonon anharmonicity is reflected by the enhancement of root mean-square displacement values. The reported giant augmentation of  $\kappa$  may inspire intensive research on auxetic carbon crystals as potential materials for emerging nanoelectronic devices.

**CARBON 122, 374-380, 2017. DOI: 10.1016/j.carbon.2017.06.100**

#### [P234-2017] “Graphene-Titanium Interfaces from Molecular Dynamics Simulations”

Fonseca, A. G.\*; Liang, T.; Zhang, D.; Choudhary, K.; Phillpot, S. R.; Sinnott, S. B.

Unraveling the physical and chemical properties of graphene-metal contacts is a key step toward the development of graphitic electronic nanodevices. Although many studies have revealed the way that various metals interact with graphene, few have described the structure and behavior of large pieces of graphene-metal nanostructures under different conditions. Here, we present the first classical molecular dynamics study of graphene-titanium (G-Ti) structures, with and without substrates. Physical and chemical properties of equilibrium structures of G-Ti interfaces with different amounts of titanium coverage are investigated. Adhesion of Ti films on graphene is shown to be enhanced by the vacancies in graphene or the electrostatic influence of substrates. The dynamics of pristine G-Ti structures at different temperatures on planar and nonplanar substrates are investigated, and the results show that G-Ti interfaces are thermally stable, that is, not prone to any reaction toward the formation of titanium carbide.

**ACS Applied Materials and Interfaces 9[38], Pages 33288-33297, 2017. DOI: 10.1021/acsami.7b09469**

## Correções

[Co002-2017] “Production of  $\pi(0)$  and eta mesons up to high transverse momentum in pp collisions at 2.76 TeV (vol 77, 339, 2017)”

Acharya, S.; Adamova, D.; Aggarwal, M. M.; Albuquerque, D. S. D.\*; Chinellato, D. D.\*; De Souza, R. D.\*; Takahashi, J.\*; et al.  
ALICE Collaboration

**EUROPEAN PHYSICAL JOURNAL C 77[9], 586, 2017. DOI: 10.1140/epjc/s10052-017-5144-7**

[Co003-2017] “Search for dark matter in proton-proton collisions at 8 TeV with missing transverse momentum and vector boson tagged jet (vol 12, 083, 2016)”

Khachatryan, V.; Sirunyan, A. M.; Tumasyan, A.; Chinellato, J. A.\*; Tonelli Manganote, E. J.\*; et al.  
CMS Collaboration

**JOURNAL OF HIGH ENERGY PHYSICS 8, 035, 2017. DOI: 10.1007/JHEP08(2017)035**

\*Autores da comunidade IFGW  
Fonte: Web of Science on-line.

## Patentes

[Pa003-2017] “Dispositivo para o controle de qualidade de imagens do tensor de difusão, de imagens ponderadas por difusão para reconstrução de imagens de tratamentos e fibras e de outros parâmetros em ressonância magnética”

Gabriela Castellano; Eduardo Tavares Costa; Edna Marina de Souza

Número da Patente ou Registro: Agência INOVA: BR 10 2017 019121 4

Tipo: Patente de Invenção

Mês/Ano de Conclusão: 09/2017 - INPI/BBRASIL

[Pa004-2017] “Técnica e dispositivo de eliminação do espalhamento Brillouin estimulado por aplicação de uma tensão mecânica aplicado num conversor de comprimento de onda óptico”

Jorge Diego Marconi; José Manuel Chávez Boggio; Hugo Luis Fragnito

Número da Patente ou Registro: Agência INOVA: PI0401220-8

Tipo: Patente de Invenção

Mês/Ano de Conclusão: 08/2017 - INPI/BBRASIL

Fonte: SIPEX - Sistema de Informação de Pesquisa e Extensão da Unicamp.

## Defesas de Teses

[T018-2017] “Estudo do impacto da moagem mecânica nas propriedades estruturais, magnéticas e magnetocatóricas de intermetálicos RM2 (R-Er, Ho, Dy e Gd; M=Al, Co)”

Aluno: Vinícius Gomes de Paula

Orientador: Prof. Dr. Lisandro Pavie Cardoso

Data: 05/10/2017

Fonte: Portal IFGW/Pós-graduação - Agenda de Colóquios, Defesas e Seminários.

Disponível em: <http://portal.ifi.unicamp.br/pos-graduacao>

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<http://abstracta.ifi.unicamp.br>

## Abstracta

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## Publicação

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