

# Abstracta

Ano XXI - N. 03

Jun-17



Artigos publicados - P071-2017 à P123-2017

Eventos publicados - P124-2017 à P125-2017

Artigos aceitos para publicação - A001-2017

Defesas de Dissertações do IFGW - D002-2017 - D005-2017

Defesas de Teses do IFGW - T009-2017 à T015-2017

## Artigos publicados

[P071-2017] “A genetic approach to the rock-paper-scissors game”

Barreto, W. P.\*; Marquitti, F. M. D.\*; de Aguiar, M. A. M.\*

Polymorphisms are usually associated with defenses and mating strategies, affecting the individual's fitness. Coexistence of different morphs is, therefore, not expected, since the fittest morph should outcompete the others. Nevertheless, coexistence is observed in many natural systems. For instance, males of the side-blotched lizards (*Uta stansburiana*) present three morphs with throat colors orange, yellow and blue, which are associated with mating strategies and territorial behavior. The three male morphs compete for females in a system that is well described by the rock-paper-scissors dynamics of game theory. Previous studies have modeled the lizards as hermaphroditic populations whose individual's behavior were determined only by their phenotypes. Here we consider an extension of this dynamical system where diploidy and sexual reproduction are explicitly taken into account. Similarly to the lizards we represent the genetic system by a single locus with three alleles, *o*, *y*, and *b* in a diploid chromosome with dominance of *o* over *y* and of *y* over *b*. We show that this genotypic description of the dynamics results in the same equilibrium phenotype frequencies as the phenotypic models, but affects the stability of the system, changing the parameter region where coexistence of the three morphs is possible in a rock-paper-scissors game.

JOURNAL OF THEORETICAL BIOLOGY 421, 146-152, 2017.  
DOI: 10.1016/j.jtbi.2017.04.003

[P072-2017] “A new approach for electron microprobe zircon fission track thermochronology”

Dias, A. N. C.; Chemale, F., Jr.; Soares, C. J.; Guedes, S.\*

Fission track thermochronology (FTT) has been applied for decades to quantify rates and timing of processes in the shallow crust. The most widely used approach is the external detector method (EDM). In this conventional approach, an age is obtained by counting both the fossil (U-238 spontaneous fission) and the induced (U-235 induced fission) tracks using an optical microscope. The induced tracks are obtained through the irradiation of the sample with thermal neutrons in the nuclear reactor, which causes fission of U-235. Based on the studies carried out by Gombosi et al. (2014), we present an alternative method of dating zircons using electron probe microprobe analysis (EPMA) to measure uranium concentration [U]. The electron microprobe analysis fission track (EPMA-FT) method was applied to three samples of rapidly cooled zircons: the Fish Canyon Tuff, Pocos de Caldas (syenite) and Serra Geral zircons. The analyses were performed using two approaches: 1) using the age equation described in Gombosi et al. (2014) and 2) using a new age equation calibration developed for this work. The results using the Gombosi et al. (2014) age equation were 26.7 +/- 4.1 Ma, 80.6 +/- 12.8 Ma and 130.9 +/- 20.1 Ma, respectively, and the results using the age equation from this work were 27.8 +/- 1.9 Ma, 83.8 +/- 7.7 Ma and 136 +/- 12 Ma, respectively. The uncertainty of the age is affected mainly by U-238 concentration and *ps* (the spontaneous fission track density) determinations. Other factors can affect the uncertainty of the age, but their contributions are smaller. For all samples, the yield ages found by the two methods are consistent and overlap within two standard deviations of published reference ages determined from other radiometric techniques (i.e., K/Ar, Ar-40/Ar-39, and/or U/Pb) and traditional FIT by the EDM.

CHEMICAL GEOLOGY 459, 129-136, 2017. DOI: 10.1016/j.chemgeo.2017.04.014

[P073-2017] “Amphiphilic Nucleating Agents to Enhance Calcium Phosphate Growth on Polymeric Surfaces”

da Silva, L. C. E.; Mas, B. A.; Duek, E. A. R.; Landers, R.\*; Bertran, C. A.; Goncalves, M. C.

Poly(epsilon-caprolactone) (PCL) is an aliphatic polyester widely explored in the preparation of guided bone regeneration (GBR) membranes because of its interesting mechanical properties and biodegradability. However, PCL high hydrophobicity often impairs cell adhesion and proliferation as well as calcium phosphate growth, all of which are crucial to achieving suitable bone tissue integration. In this work, aimed at achieving less-hydrophobic surfaces, amphiphilic molecules were added at low concentrations to the polymeric dope solutions that generated the GBR membranes. During membrane formation, these molecules migrate to the solution/air interface in such a way that, upon liquid solid phase transition, the negatively charged heads are exposed while the apolar tails are anchored to the polymer bulk. As a consequence, these molecules became nucleating agents for subsequent calcium phosphate growth using an alternating soaking process. Herein, PCL porous membranes containing different amphiphilic molecules, such as stearic acid and bis(2,ethylhexyl) phosphate, were investigated. This new, simple, and atoxic method to superficially treat polymeric membranes could be extended to a wide range of polymers and applications.

LANGMUIR 33[15], 3855-3863, 2017. DOI: 10.1021/acs.langmuir.6b04562

[P074-2017] “An experimental and theoretical investigation into the electronically excited states of para-benzoquinone”

Jones, D. B.; Limao-Vieira, P.; Mendes, M.; Jones, N. C.; Hoffmann, S. V.; da Costa, R. F.\*; Varella, M. T. do N.; Bettega, M. H. F.; Blanco, F.; Garcia, G.; Ingolfsson, O.; Lima, M. A. P.\*; Brunger, M. J.

We report on a combination of experimental and theoretical investigations into the structure of electronically excited para-benzoquinone (pBQ). Here synchrotron photoabsorption measurements are reported over the 4.0-10.8 eV range. The higher resolution obtained reveals previously unresolved pBQ spectral features. Time-dependent density functional theory calculations are used to interpret the spectrum and resolve discrepancies relating to the interpretation of the Rydberg progressions. Electron-impact energy loss experiments are also reported. These are combined with elastic electron scattering cross section calculations performed within the framework of the independent atom model-screening corrected additivity rule plus interference (IAM-SCAR + I) method to derive differential cross sections for electronic excitation of key spectral bands. A generalized oscillator strength analysis is also performed, with the obtained results demonstrating that a cohesive and reliable quantum chemical structure and cross section framework has been established. Within this context, we also discuss some issues associated with the development of a minimal orbital basis for the single configuration interaction strategy to be used for our high-level low-energy electron scattering calculations that will be carried out as a subsequent step in this joint experimental and theoretical investigation.

JOURNAL OF CHEMICAL PHYSICS 146[18], 184303, 2017.  
DOI: 10.1063/1.4982940

[P075-2017] “Annealing effects on the structural and optical properties of vanadium oxide film obtained by the hot-filament metal oxide deposition technique (HFMOD)”

Scarmínio, J.; Catarini da Silva, P. R.; Gelamo, R. V.; Bica de Moraes, M. A.\*



Vanadium oxide films amorphous, nonstoichiometric and highly absorbing in the optical region were deposited on ITO-coated glass and on silicon substrates, by the hot-filament metal oxide deposition technique (HFMOD) and oxidized by ex-situ annealing in a furnace at 200, 300, 400 and 500 degrees C, under an atmosphere of argon and rarefied oxygen. X-ray diffraction, Raman and Rutherford backscattering spectroscopy as well as optical transmission were employed to characterize the amorphous and annealed films. When annealed at 200 and 300 degrees C the as-deposited opaque films become transparent but still amorphous. Under treatments at 400 and 500 degrees C a crystalline nonstoichiometric V2O5 structure is formed. All the annealed films became semiconducting, with their optical absorption coefficients changing with the annealing temperature. An optical gap of 2.25 eV was measured for the films annealed at 400 and 500 degrees C. The annealing in rarefied oxygen atmosphere proved to be a useful and simple ex-situ method to modulate the structural and optical properties of vanadium oxide films deposited by HFMOD technique. This technique could be applied to other amorphous and non-absorbing oxide films, replacing the conventional and sometimes expensive method of modulate desirable film properties by controlling the film deposition parameters. Even more, the HFMOD technique can be an inexpensive alternative to deposit metal oxide films.

**MATERIA-RIO DE JANEIRO 22[1], UNSP e11781, 2017. DOI: 10.1590/S1517-707620170001.0113**

**[P076-2017] “Changes in Properties of Dielectric Barrier Discharge Plasma Jets for Different Gases and for Insulating and Conducting Transfer Plates”**

do Nascimento, F.; Moshkalev, S.; Machida, M.\*

Dielectric barrier discharge (DBD) plasma jets have been studied extensively in recent years because of its wide range of applications. DBD plasmas can be produced using many different gases and can be applied to a broad variety of surfaces and substrates. This work provides comparisons of DBD plasmas generated using argon (Ar), helium (He), and nitrogen (N<sub>2</sub>), as well as their mixtures with water vapor in order to know how some plasma properties are affected by the use of different gases. All plasmas were studied in two different conditions: using a transfer plate made of a conductive material and using a transfer plate made of an insulating one. It was observed that the process of Penning ionization of nitrogen molecules by direct collisions with metastable atoms and molecules is evident and significant only in plasmas that use He as the working gas, which means that He atoms in metastable states have greater ability to transfer energy to molecules of nitrogen in the plasma. The collisions of metastable He with N<sub>2</sub> molecules determine the vibrational temperature (T (vib)) values in He plasmas, while in Ar and N<sub>2</sub> plasmas, the T (vib) values are determined mainly by collisions of electrons with N<sub>2</sub> molecules. It was noticed that the use of an insulating or a conducting transfer plate as the sample holder affects the results of adhesion between poly(dimethylsiloxane) samples, and it is mainly due to the differences in the plasma power, with a higher plasma power leading to better adhesion.

**BRAZILIAN JOURNAL OF PHYSICS 47[3], 278-287, 2017. DOI: 10.1007/s13538-017-0492-1**

**[P077-2017] “Charged-particle multiplicities in proton-proton collisions at root s=0.9 to 8 TeV”**

Adam, J.; Adamova, D.; Aggarwal, M. M.; Chinellato, D. D.\*; Dash, A.\*; Takahashi, J.\*; et al.  
ALICE Collaboration

A detailed study of pseudorapidity densities and multiplicity distributions of primary charged particles produced in proton-proton collisions, at  $\sqrt{s} = 0.9, 2.36, 2.76, 7$  and  $8$  TeV, in the pseudorapidity range  $|\eta| < 2$ , was carried out using the ALICE detector. Measurements were obtained for three event classes: inelastic, non-single diffractive and events with at least one charged particle in the pseudorapidity interval  $|\eta| < 1$ . The use of an improved track-counting algorithm combined with ALICE's measurements of diffractive processes allows a higher precision compared to our previous publications. A KNO scaling study was performed in the pseudorapidity intervals  $|\eta| < 0.5, 1.0$  and  $1.5$ . The data are compared to other experimental results and to models as implemented in Monte Carlo event generators PHOJET and recent tunes of PYTHIA6, PYTHIA8 and EPOS.

**EUROPEAN PHYSICAL JOURNAL C 77[1], 33, 2017. DOI: 10.1140/epjc/s10052-016-4571-1**

**[P078-2017] “Charged-particle nuclear modification factors in PbPb and pPb collisions at root s(NN)=5.02 TeV”**

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

The spectra of charged particles produced within the pseudorapidity window  $|\eta| < 1$  at  $\sqrt{s(NN)} = 5.02$  TeV are measured using  $404 \mu\text{b}^{-1}$  of PbPb and  $27.4 \text{pb}^{-1}$  of pp data collected by the CMS detector at the LHC in 2015. The spectra are presented over the transverse momentum ranges spanning  $0 < p(T) < 400$  GeV in pp and  $0 < p(T) < 400$  GeV in PbPb collisions. The corresponding nuclear modification factor, R-AA, is measured in bins of collision centrality. The R-AA in the 5% most central collisions shows a maximal suppression by a factor of 7-8 in the  $p(T)$  region of 6-9 GeV. This dip is followed by an increase, which continues up to the highest  $p(T)$  measured, and approaches unity in the vicinity of  $p(T) = 200$  GeV. The R-AA is compared to theoretical predictions and earlier experimental results at lower collision energies. The newly measured pp spectrum is combined with the pPb spectrum previously published by the CMS collaboration to construct the pPb nuclear modification factor, R-pA, up to 120 GeV. For  $p(T) > 20$  GeV, R-pA exhibits weak momentum dependence and shows a moderate enhancement above unity.

**JOURNAL OF HIGH ENERGY PHYSICS 4, 039, 2017. DOI: 10.1007/JHEP04(2017)039**

**[P079-2017] “Computational Modeling for the Ag Nanoparticle Coalescence Process: A Case of Surface Plasmon Resonance”**

Faccin, G. M.; San-Miguel, M. A.; Andres, J.; Longo, E.; da Silva, E. Z.\*

Motivated by recent transmission electron microscopy (TEM) experiments on alpha-Ag<sub>2</sub>WO<sub>4</sub>, the coalescence process of Ag nanoparticles (NPs) is investigated using molecular dynamics (MD) simulations. These Ag NPs are formed by irradiation of alpha-Ag<sub>2</sub>WO<sub>4</sub> crystals by electrons from a TEM gun. This behavior can be considered as a clear example of surface plasmon resonance (SPR), in which Ag NP coalescence processes are controlled by dipole-dipole interaction forming larger clusters. The interactions between Ag NPs along the coalescence processes are studied using MD simulations with embedded atom method (EAM) effective potentials for Ag. With these choices of methods, coalescence is studied by addressing different scenarios for the interacting NPs, which all could possibly occur in experiments.

**JOURNAL OF PHYSICAL CHEMISTRY C 121[12], 7030-7036, 2017. DOI: 10.1021/acs.jpcc.7b00769**

**[P080-2017] “Cosmic-muon characterization and annual modulation measurement with Double Chooz detectors”**

Abrahamo, T.; Almazan, H.; dos Anjos, J. C.; Kemp, E.\*; et al.  
Double Chooz Collaboration

A study on cosmic muons has been performed for the two identical near and far neutrino detectors of the Double Chooz experiment, placed at similar to 120 and similar to 300 m. w.e. underground respectively, including the corresponding simulations using the MUSIC simulation package. This characterization has allowed us to measure the muon flux reaching both detectors to be  $(3.64 \pm 0.04) \times 10^{-4} \text{ cm}^{-2} \text{ s}^{-1}$  for the near detector and  $(7.00 \pm 0.05) \times 10^{-5} \text{ cm}^{-2} \text{ s}^{-1}$  for the far one. The seasonal modulation of the signal has also been studied observing a positive correlation with the atmospheric temperature, leading to an effective temperature coefficient of  $\alpha(T) = 0.212 \pm 0.024$  and  $0.355 \pm 0.019$  for the near and far detectors respectively. These measurements, in good agreement with expectations based on theoretical models, represent one of the first measurements of this coefficient in shallow depth installations.

**JOURNAL OF COSMOLOGY AND ASTROPARTICLE PHYSICS 2, 017, 2017. DOI: 10.1088/1475-7516/2017/02/017**

**[P081-2017] “Crystal field effects in the intermetallic RNi<sub>3</sub>Ga<sub>9</sub> (R = Tb, Dy, Ho, and Er) compounds”**

Silva, L. S.; Mercena, S. G.; Garcia, D. J.; Bittar, E. M.; Jesus, C. B. R.\*; Pagliuso, P. G.\*; Lora-Serrano, R.; Meneses, C. T.; Duque, J. G. S.\*

In this paper, we report temperature-dependent magnetic susceptibility, electrical resistivity, and heat-capacity experiments in the family of intermetallic compounds RNi<sub>3</sub>Ga<sub>9</sub> (R = Tb, Dy, Ho, and Er). Single-crystalline samples were grown using Ga self-flux method. These materials crystallize in a trigonal RNi<sub>3</sub>Al<sub>9</sub>-type structure with space group R32. They all order antiferromagnetically with T-N < 20 K. The anisotropic magnetic susceptibility presents large values of the ratio  $\chi(\text{easy}) / \chi(\text{hard})$  indicating strong crystalline electric-field (CEF) effects. The evolution of the crystal-field scheme for each R was analyzed in detail by using a spin model including anisotropic nearest-neighbor Ruderman-Kittel-Kasuya-Yosida interaction and the trigonal CEF Hamiltonian. Our analysis allows one to understand the distinct direction of the ordered moments along the series-the Tb-, Dy-, and Ho-based compounds have the ordered magnetic moments in the easy ab plane and the Er sample magnetization easy axis is along the  $\langle c \rangle$  direction.

**PHYSICAL REVIEW B 95[13], 134434, 2017. DOI: 10.1103/PhysRevB.95.134434**

**[P082-2017] “Density functional investigation of the adsorption effects of PH<sub>3</sub> and SH<sub>2</sub> on the structure stability of the Au-55 and Pt-55 nanoclusters”**

Guedes-Sobrinho, D.; Chaves, A. S.\*; Piotrowski, M. J.; Da Silva, J. L. F.

Although several studies have been reported for Pt-55 and Au-55 nanoclusters, our atomistic understanding of the interplay between the adsorbate-surface interactions and the mechanisms that lead to the formation of the distorted reduced core (DRC) structures, instead of the icosahedron (ICO) structure in gas phase, is still far from satisfactory. Here, we report a density functional theory (DFT) investigation of the role of the adsorption effects of PH<sub>3</sub> (one lone pair of electrons) and SH<sub>2</sub> (two lone pairs) on the relative stability of the Pt-55 and Au-55 nanoclusters. In gas phase, we found that the DRC structures with 7 and 9 atoms in the core region are about 5.34 eV (Pt-55) and 2.20 eV (Au-55) lower in energy than the ICO model with I-h symmetry and 13 atoms in the core region.

However, the stability of the ICO structure increases by increasing the number of adsorbed molecules from 1 to 18, in which both DRC and ICO structures are nearly degenerate in energy at the limit of 18 ligands, which can be explained as follows. In gas phase, there is a strong compression of the cationic core region by the anionic surface atoms induced by the attractive Coulomb interactions (core(+)-surface(-)), and hence, the strain release is obtained by reducing the number of atoms in the cationic core region, which leads to the 55 atoms distorted reduced core structures. Thus, the Coulomb interactions between the core(+) and surface(-) contribute to break the symmetry in the ICO55 structure. On the other hand, the addition of ligands on the anionic surface reduces the charge transfer between the core and surface, which contributes to decrease the Coulomb interactions and the strain on the core region of the ICO structure, and hence, it stabilizes a compact ICO structure. The same conclusion is obtained by adding van der Waals corrections to the plain DFT calculations. Similar results are obtained by the addition of steric effects, which are considered through the adsorption of triphenylphosphine (PPh<sub>3</sub>) molecules on Au-55, in which the relative stability between ICO and DRC is the same as for PH<sub>3</sub> and SH<sub>2</sub>. However, for Pt-55, we found an inversion of stability due to the PPh<sub>3</sub> ligand effects, where ICO has higher stability than DRC by 2.40 eV. Our insights are supported by several structural, electronic, and energetic analyses.

**JOURNAL OF CHEMICAL PHYSICS 146[16], 164304, 2017. DOI: 10.1063/1.4981791**

**[P083-2017] “Direct Drawing Method of Graphite onto Paper for High-Performance Flexible Electrochemical Sensors”**

Santhiago, M.; Strauss, M.; Pereira, M. P.; Chagas, A. S.; Bufon, C. C. B.\*

A simple and fast fabrication method to create high-performance pencil-drawn electrochemical sensors is reported for the first time. The sluggish electron-transfer observed on bare pencil-drawn surfaces was enhanced using two electrochemical steps: first oxidizing the surface and then reducing it in a subsequent step. The heterogeneous rate constant was found to be  $5.1 \times 10^{-3} \text{ cm s}^{-1}$ , which is the highest value reported so far for pencil-drawn surfaces. We mapped the origin of such performance by atomic force microscopy, X-ray photoelectron spectroscopy, and Raman spectroscopy.- Our results suggest that the oxidation process leads to ‘chemical and structural transformations on the surface. As a proof-of-concept, we modified the pencil-drawn surface with, Meldola’s blue to electrocatalytically detect nicotinamide adenine dinucleotide (NADH). The electrochemical device exhibited the highest catalytic constant  $41.7 \times 10^5 \text{ L mol}^{-1} \text{ s}^{-1}$ ) and the lowest detection potential for NADH reported so far in paper-based electrodes.

**ACS APPLIED MATERIALS & INTERFACES 9[13], 11959-11966, 2017. DOI: 10.1021/acsami.6b15646**

**[P084-2017] “Domain wall propagation tuning in magnetic nanowires through geometric modulation”**

Arzuza, L. C. C.\*; Lopez-Ruiz, R.\*; Salazar-Aravena, D.\*; Knobel, M.\*; Beron, F.\*; Pirota, K. R.\*

The magnetic behavior of nickel modulated nanowires embedded in porous alumina membranes is investigated. Their diameters exhibit a sharp transition between below (35 nm) and above (52 nm) the theoretical limit for transverse and vortex domain walls. Magnetic hysteresis loops and first-order reversal curves (FORCs) were measured on several ordered nanowire arrays with different wide-narrow segment lengths ratio and compared with those from homogenous nanowires.

The experimental magnetic response evidences a rather complex susceptibility behavior for nanowires with modulated diameter. Micromagnetic simulations on isolated and first-neighbors arrays of nanowires show that the domain wall structure, which depends on the segment diameter, suffers a transformation while crossing the diameter modulation, but without any pinning. The experimental array magnetic behavior can be ascribed to a heterogeneous stray field induced by the diameter modulation, yielding a stronger interaction field at the wide extremity than at the narrow one. The results evidence the possibility to control the domain wall propagation and morphology by modulating the lateral aspect of the magnetic entity.

**JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS 432, 309-317, 2017. DOI: 10.1016/j.jmmm.2017.01.071**

**[P085-2017] "Evidence of phase transitions in MoO<sub>2</sub> single crystals"**

Alves, L. M. S.; Oliveira, F. S.; de Lima, B. S.; da Luz, M. S.; Rebello, A.; Masunaga, S. H.; Neumeier, J. J.; Giles, C.\*; Leao, J. B.; dos Santos, C. A. M.

In this work, structural and physical properties are revisited in the MoO<sub>2</sub> compound. MoO<sub>2</sub> single crystals have been prepared by chemical vapor transport technique and characterized by X-ray diffraction, neutron diffraction, high-resolution thermal expansion, electrical resistance measurements, and heat capacity. Electrical resistivity, heat capacity, and thermal expansion measurements show two clear features which are related to phase transitions on the MoO<sub>2</sub> compound. These results suggest that an electronic-type transition occurs near 220 K and a structural transition at similar to 267 K.

**JOURNAL OF ALLOYS AND COMPOUNDS 705, 764-768, 2017. DOI: 10.1016/j.jallcom.2017.02.148**

**[P086-2017] "Flow Dominance and Factorization of Transverse Momentum Correlations in Pb-Pb Collisions at the LHC"**

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

We present the first measurement of the two-particle transverse momentum differential correlation function,  $P_2 = \langle \Delta p_T \Delta p(T) \rangle / \langle p(T) \rangle^2$ , in Pb-Pb collisions at  $\sqrt{s(NN)} = 2.76$  TeV. Results for  $P_2$  are reported as a function of the relative pseudorapidity ( $\Delta \eta$ ) and azimuthal angle ( $\Delta \phi$ ) between two particles for different collision centralities. The  $\Delta \phi$  dependence is found to be largely independent of  $\Delta \eta$  for broken vertical bar  $\Delta \eta$  broken vertical bar  $\geq 0.9$ . In the 5% most central Pb-Pb collisions, the two-particle transverse momentum correlation function exhibits a clear double-hump structure around  $\Delta \phi = \pi$  (i. e., on the away side), which is not observed in number correlations in the same centrality range, and thus provides an indication of the dominance of triangular flow in this collision centrality. Fourier decompositions of  $P_2$ , studied as a function of the collision centrality, show that correlations at broken vertical bar  $\Delta \eta$  broken vertical bar  $\geq 0.9$  can be well reproduced by a flow ansatz based on the notion that measured transverse momentum correlations are strictly determined by the collective motion of the system.

**PHYSICAL REVIEW LETTERS 118[16], 162302, 2017. DOI: 10.1103/PhysRevLett.118.162302**

**[P087-2017] "Formation of Rh islands on Pd-supported alpha-Fe<sub>2</sub>O<sub>3</sub> (0001)"**

Pancotti, A.; Abreu, G. J. P.; Wang, J. L.; Ferreira, A. V. M.; Landers, R.\*; de Siervo, A.\*

A rhodium ultra-thin film was deposited on a Pd-supported alpha-Fe<sub>2</sub>O<sub>3</sub> (0001) film by molecular beam epitaxy (MBE). The surface atomic and electronic structures were studied using X-ray photoelectron diffraction (XPD), X-ray photoelectron spectroscopy (XPS), and low energy electron diffraction (LEED). For an oxide thin film (similar to 16.5 angstrom), an ordered (root 3 x root 3)R30 degrees structure was observed. The multiple scattering calculation approach combined with a genetic algorithm for surface structure optimization was used to investigate precisely the atomic structure of the oxide support as well as the Rh nanoislands or nanoparticles (NPs). Rh exhibited 3D growth on an alpha-Fe<sub>2</sub>O<sub>3</sub> thin film forming NPs with a lattice constant expanded by 5.26% relative to the Rh bulk value. The coexistence of 60 degrees rotated domains and also evidence of Fe termination at the surface of alpha-Fe<sub>2</sub>O<sub>3</sub> were observed.

**CRYSTENGCOMM 19[15], 2089-2095, 2017. DOI: 10.1039/c6ce02485h**

**[P088-2017] "Formation of solitary waves and oscillatory shocklets in a two-temperature electron kappa-distributed plasma"**

Naeem, I.; Ali, S.; Sakanaka, P. H.\*; Mirza, A. M.

Large-amplitude electron acoustic (EA) waves and shocklets are investigated in a two-temperature electron plasma. For this purpose, dynamical cold electrons are described by the fully nonlinear continuity and momentum equations, while superthermal (hot) inertialess electrons are described by the kappa-distribution function with a neutralizing background of static positive ions. The fluid equations along with a quasineutrality equation are solved to obtain a set of two characteristic wave equations that admit analytical and numerical solutions. It is shown that variation due to hot electron superthermality and hot-to-cold electron density ratio strongly affects the profiles of nonlinear EA structures in terms of negative potential, cold electron velocity and density. In particular, at time  $\tau = 0$ ; symmetric solitary pulses are formed, which develop into oscillatory shocklets with the course of time. Our results should be useful for understanding solitary excitations and associated nonstationary large-amplitude shocklets in laboratory kappa-distributed plasmas, where superthermal (hot) energetic electrons exist.

**PHYSICS OF PLASMAS 24[4], 042109, 2017. DOI: 10.1063/1.4979675**

**[P089-2017] "High Toughness in Ultralow Density Graphene Oxide Foam"**

Owuor, P. S.; Woellner, C. F.\*; Li, T.; Vinod, S.; Ozden, S.; Kosolwattana, S.; Bhowmick, S.; Duy, L. X.; Salvatierra, R. V.; Wei, B.; Asif, S. A. S.; Tour, J. M.; Vajtai, R.; Lou, J.; Galvao, D. S.\*; Tiwary, C. S.; Ajayan, P. M.

Here, the scalable synthesis of low-density 3D macroscopic structure of graphene oxide (GO) interconnected with polydimethylsiloxane (PDMS) is reported. A controlled amount of PDMS is infused into the freeze-dried foam to result into a very rigid structure with improved mechanical properties, such as tensile plasticity and toughness. The PDMS wets the graphene oxide sheets and acts like glue between the 2D sheets. Molecular dynamics simulations are used to further elucidate the mechanisms of the interactions of graphene oxide layers with PDMS. The ability of using the interconnecting graphene oxide foam as an effective oil-water separator and stable insulating behavior to elevated temperatures are further demonstrated. The structural rigidity of the sample is also tested using laser impact and compared with GO foam.



ADVANCED MATERIALS INTERFACES 4[10], 1700030, 2017. DOI: 10.1002/admi.201700030

[P090-2017] “Integration of bow-tie plasmonic nano-antennas on tapered fibers”

Khaleque, A.; Mironov, E. G.; Osorio, J. H.\*; Li, Z.; Cordeiro, C. M. B.\*; Liu, L.; Franco, M. A. R.; Liow, J. L.; Hattori, H. T.

In this article, a new and flexible approach to control the electric field enhancement of bow-tie nano-antennas by integrating them on the lateral of a tapered optical fiber is proposed. The device is driven by a Q-switched laser and the performance of a fabricated nano-antenna in a quartz slide is tested by a Surface Enhanced Raman Scattering (SERS) experiment. A refractive index sensing experiment is also performed and a sensitivity of  $(240 \pm 30)$  nm/RIU is found in the 1.33-1.35 index range.

OPTICS EXPRESS 25[8], 8986-8996, 2017. DOI: 10.1364/OE.25.008986

[P091-2017] “Measurement and QCD analysis of double-differential inclusive jet cross sections in pp collisions at root s=8 TeV and cross section ratios to 2.76 and 7 TeV”

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

A measurement of the double-differential inclusive jet cross section as a function of the jet transverse momentum  $p(T)$  and the absolute jet rapidity  $|y|$  is presented. Data from LHC proton-proton collisions at root  $s = 8$  TeV, corresponding to an integrated luminosity of  $19.7 \text{ fb}^{-1}$ , have been collected with the CMS detector. Jets are reconstructed using the anti- $k(T)$  clustering algorithm with a size parameter of 0.7 in a phase space region covering jet  $p(T)$  from 74 GeV up to 2.5 TeV and jet absolute rapidity up to  $|y| = 3.0$ . The low- $p(T)$  jet range between 21 and 74 GeV is also studied up to  $|y| = 4.7$ , using a dedicated data sample corresponding to an integrated luminosity of  $5.6 \text{ pb}^{-1}$ . The measured jet cross section is corrected for detector effects and compared with the predictions from perturbative QCD at next-to-leading order (NLO) using various sets of parton distribution functions (PDF). Cross section ratios to the corresponding measurements performed at 2.76 and 7 TeV are presented. From the measured double-differential jet cross section, the value of the strong coupling constant evaluated at the Z mass is  $\alpha(S)(M-Z) = 0.1164(-0.0043)(+0.0060)$ , where the errors include the PDF, scale, nonperturbative effects and experimental uncertainties, using the CT10 NLO PDFs. Improved constraints on PDFs based on the inclusive jet cross section measurement are presented.

JOURNAL OF HIGH ENERGY PHYSICS 3, 156, 2017. DOI: 10.1007/JHEP03(2017)156

[P092-2017] “Measurement of azimuthal correlations of D mesons with charged particles in pp collisions at root s=7 TeV and p-Pb collisions at root(sNN)-N-s=5.02 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 azimuthal correlations of D mesons with charged particles were measured with the ALICE apparatus in pp collisions at root  $s = 7$  TeV and p-Pb collisions at root  $s_{NN} = 5.02$  TeV at the Large Hadron Collider.  $D^0$ ,  $D^+$ , and  $D^{*+}$  mesons and their charge conjugates with transverse momentum  $3 < p_T < 16$  GeV/c and rapidity in the nucleon-nucleon centre-of-mass system vertical bar  $y(\text{cms})$  vertical bar  $< 0.5$  (pp collisions)

and  $-0.96 < y(\text{cms}) < 0.04$  (p-Pb collisions) were correlated to charged particles with  $p(T) > 0.3$  GeV/c. The yield of charged particles in the correlation peak induced by the jet containing the D meson and the peak width are compatible within uncertainties in the two collision systems. The data are described within uncertainties by Monte-Carlo simulations based on PYTHIA, POWHEG, and EPOS 3 event generators.

EUROPEAN PHYSICAL JOURNAL C 77[4], 245, 2017. DOI: 10.1140/epjc/s10052-017-4779-8

[P093-2017] “Measurement of differential cross sections for top quark pair production using the lepton plus jets final state in proton-proton collisions at 13 TeV”

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

Differential and double-differential cross sections for the production of top quark pairs in proton-proton collisions at 13 TeV are measured as a function of jet multiplicity and of kinematic variables of the top quarks and the top quark-antiquark system. This analysis is based on data collected by the CMS experiment at the LHC corresponding to an integrated luminosity of  $2.3 \text{ fb}^{-1}$ . The measurements are performed in the lepton + jets decay channels with a single muon or electron in the final state. The differential cross sections are presented at particle level, within a phase space close to the experimental acceptance, and at parton level in the full phase space. The results are compared to several standard model predictions.

PHYSICAL REVIEW D 95[9], 092001, 2017. DOI: 10.1103/PhysRevD.95.092001

[P094-2017] “Measurement of prompt and nonprompt J/psi production in pp and pPb 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

This paper reports the measurement of J/psi meson production in proton proton (pp) and proton lead (pPb) collisions at a center-of-mass energy per nucleon pair of 5.02 TeV by the CMS experiment at the LHC. The data samples used in the analysis correspond to integrated luminosities of  $28 \text{ pb}^{-1}$  and  $35 \text{ nb}^{-1}$  for pp and pPb collisions, respectively. Prompt and nonprompt J/psi mesons, the latter produced in the decay of B hadrons, are measured in their dilution decay channels. Differential cross sections are measured in the transverse momentum range of  $2 < p(T) < 30$  GeV/c, and center-of-mass rapidity ranges of vertical bar  $y(\text{CM})$  vertical bar  $< 2.4$  (pp) and  $-2.87 < y(\text{CM}) < 1.93$  (pPb). The nuclear modification factor,  $R_{pPb}$ , is measured as a function of both  $p(T)$  and  $y(\text{CM})$ . Small modifications to the J/psi cross sections are observed in pPb relative to pp collisions. The ratio of J/psi production cross sections in p-going and Pb-going directions,  $R_{\text{FB}}$ , studied as functions of  $p(T)$  and  $y(\text{CM})$ , shows a significant decrease for increasing transverse energy deposited at large pseudorapidities. These results, which cover a wide kinematic range, provide new insight on the role of cold nuclear matter effects on prompt and nonprompt J/psi production.

EUROPEAN PHYSICAL JOURNAL C 77[4], 269, 2017. DOI: 10.1140/epjc/s10052-017-4828-3

[P095-2017] “Measurement of the production cross section of a W boson in association with two b jets in pp collisions at root s=8TeV”

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

The production cross section of a W boson in association with two b jets is measured using a sample of proton-proton collisions at  $\sqrt{s} = 8$  TeV collected by the CMS experiment at the CERN LHC. The data sample corresponds to an integrated luminosity of  $19.8 \text{ fb}^{-1}$ . The W bosons are reconstructed via their leptonic decays,  $W \rightarrow l(\nu)$  where  $l = \mu$  or  $e$ . The fiducial region studied contains exactly one lepton with transverse momentum  $p_T(l) > 30$  GeV and pseudorapidity  $|\eta(l)| < 2.1$ , with exactly two b jets with  $p_T > 25$  GeV and  $|\eta(l)| < 2.4$  and no other jets with  $p_T > 25$  GeV and  $|\eta(l)| < 4.7$ . The cross section is measured to be  $\sigma(\text{pp} \rightarrow W(l\nu)+b\bar{c}(\text{b over bar})\bar{c}) = 0.64 \pm 0.03$  (stat)  $\pm 0.10$  (syst)  $\pm 0.06$  (theo)  $\pm 0.02$  (lumi) pb, in agreement with standard model predictions.

EUROPEAN PHYSICAL JOURNAL C 77[2], 92, 2017. DOI: 10.1140/epjc/s10052-016-4573-z.

[P096-2017] “Measurement of the  $t(\bar{t})$  production cross section using events in the  $e \mu$  final state 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 cross section of top quark-antiquark pair production in proton-proton collisions at  $\sqrt{s} = 13$  TeV is measured by the CMS experiment at the LHC, using data corresponding to an integrated luminosity of  $2.2 \text{ fb}^{-1}$ . The measurement is performed by analyzing events in which the final state includes one electron, one muon, and two or more jets, at least one of which is identified as originating from hadronization of a b quark. The measured cross section is  $815 \pm 9$  (stat)  $\pm 38$  (syst)  $\pm 19$  (lumi) pb, in agreement with the expectation from the standard model.

EUROPEAN PHYSICAL JOURNAL C 77[3], 172, 2017. DOI: 10.1140/epjc/s10052-017-4718-8

[P097-2017] “Measurement of the WZ production cross section in pp collisions at  $\sqrt{s}=7$  and 8 TeV and search for anomalous triple gauge couplings at  $\sqrt{s}=8$  TeV”

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

The WZ production cross section is measured by the CMS experiment at the CERN LHC in proton proton collision data samples corresponding to integrated luminosities of  $4.9 \text{ fb}^{-1}$  collected at  $\sqrt{s} = 7$  TeV, and  $19.6 \text{ fb}^{-1}$  at  $\sqrt{s} = 8$  TeV. The measurements are performed using the fully-leptonic WZ decay modes with electrons and muons in the final state. The measured cross sections for  $71 < m(Z) < 111$  GeV are  $\sigma(\text{pp} \rightarrow WZ; \sqrt{s} = 7 \text{ TeV}) = 20.14 \pm 1.32$  (stat)  $\pm 0.38$  (theo)  $\pm 1.06$  (exp)  $\pm 0.44$  (lumi) pb and  $\sigma(\text{pp} \rightarrow WZ; \sqrt{s} = 8 \text{ TeV}) = 24.09 \pm 0.87$  (stat)  $0.80$  (theo)  $\pm 1.40$  (exp)  $\pm 0.63$  (lumi) pb. Differential cross sections with respect to the Z boson  $p(T)$ , the leading jet  $p(T)$ , and the number of jets are obtained using the  $\sqrt{s} = 8$  TeV data. The results are consistent with standard model predictions and constraints on anomalous triple gauge couplings are obtained.

EUROPEAN PHYSICAL JOURNAL C 77[4], 236, 2017. DOI: 10.1140/epjc/s10052-017-4730-z

[P098-2017] “Measurements of differential production cross sections for a Z boson in association with jets in pp collisions at  $\sqrt{s}=8$  TeV”

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

Cross sections for the production of a Z boson in association with jets in proton-proton collisions at a centre-of-mass energy of  $\sqrt{s} = 8$  TeV are measured using a data sample collected by the CMS experiment at the LHC corresponding to  $19.6 \text{ fb}^{-1}$ . Differential cross sections are presented as functions of up to three observables that describe the jet kinematics and the jet activity. Correlations between the azimuthal directions and the rapidities of the jets and the Z boson are studied in detail. The predictions of a number of multileg generators with leading or next-to-leading order accuracy are compared with the measurements. The comparison shows the importance of including multi-parton contributions in the matrix elements and the improvement in the predictions when next-to-leading order terms are included.

JOURNAL OF HIGH ENERGY PHYSICS 4, 022, 2017. DOI: 10.1007/JHEP04(2017)022

[P099-2017] “Multiplicity and rapidity dependence of strange hadron production in pp, pPb, and PbPb collisions at the LHC”

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

Measurements of strange hadron ( $K_S(0)$ ,  $\Lambda$ ,  $\Lambda_b$ ,  $\Xi(0)$ ,  $\Xi_b$ ) transverse momentum spectra in pp, pPb, and PbPb collisions are presented over a wide range of rapidity and event charged-particle multiplicity. The data were collected with the CMS detector at the CERN LHC in pp collisions at  $\sqrt{s} = 7$  TeV, pPb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV, and PbPb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV. The average transverse kinetic energy is found to increase with multiplicity, at a faster rate for heavier strange particle species in all systems. At similar multiplicities, the difference in average transverse kinetic energy between different particle species is observed to be larger for pp and pPb events than for PbPb events. In pPb collisions, the average transverse kinetic energy is found to be slightly larger in the Pb-going direction than in the p-going direction for events with large multiplicity. The spectra are compared to models motivated by hydrodynamics.

PHYSICS LETTERS B 768, 103-129, 2017. DOI: 10.1016/j.physletb.2017.01.075

[P100-2017] “Nonlinear photovoltaic effect in Sillenite photorefractive crystals”

de Oliveira, I.; Capovilla, D. A.; Moura, A. L.; Timoteo, V. S.; Carvalho, J. F.; Frejlich, J.\*

We report on the presence of photovoltaic effect in some Sillenite photorefractive crystals and compare their behavior with that of the well known photovoltaic  $\text{LiNbO}_3:\text{Fe}$  crystal. Nonlinear photovoltaic behavior of these Sillenites are also reported here for the first time and explained by the presence of shallow along with deep photovoltaic centers.

OPTICAL MATERIALS 66, 72-78, 2017. DOI: 10.1016/j.optmat.2017.01.028

[P101-2017] “Note: Experimental setup for measuring the barocaloric effect in polymers: Application to natural rubber”

Bom, N. M.; Usuda, E. O.; Guimaraes, G. M.; Coelho, A. A.\*; Carvalho, A. M. G.

Barocaloric materials have shown to be promising alternatives to the conventional vapor-compression refrigeration technologies. Nevertheless, barocaloric effect ( $\sigma(b)$ -CE) has not been extensively examined for many classes of materials up to now. Aiming at fulfilling this gap, the present paper describes the development of a high-pressure experimental setup for measuring the  $\sigma(b)$ -CE in polymers. The design allows simultaneous measurements of temperature, pressure, and strain during the barocaloric cycle. The system proved to be fully functional through basic experiments using natural rubber. Samples exhibited large temperature variations associated with the  $\sigma(b)$ -CE. Strain-temperature curves were also obtained, which could allow indirect measurements of the isothermal entropy change.

REVIEW OF SCIENTIFIC INSTRUMENTS 88[4], 046103, 2017. DOI: 10.1063/1.4979464

[P102-2017] “Observation of  $\gamma(1S)$  pair production in proton-proton collisions at  $\sqrt{s}=8$  TeV”

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

Pair production of  $\gamma(1S)$  mesons is observed at the LHC in proton-proton collisions at  $\sqrt{s} = 8$  TeV by the CMS experiment in a data sample corresponding to an integrated luminosity of 20.7 fb<sup>-1</sup>. Both  $\gamma(1S)$  candidates are fully reconstructed via their decays to  $\mu^+ \mu^-$ . The fiducial acceptance region is defined by an absolute  $\gamma(1S)$  rapidity smaller than 2.0. The fiducial cross section for the production of  $\gamma(1S)$  pairs, assuming that both mesons decay isotropically, is measured to be 68.8  $\pm$  12.7 (stat)  $\pm$  7.4 (syst)  $\pm$  2.8 (B) pb, where the third uncertainty comes from the uncertainty in the branching fraction of  $\gamma(1S)$  decays to  $\mu^+ \mu^-$ . Assuming instead that the  $\gamma(1S)$  mesons are produced with different polarizations leads to variations in the measured cross section in the range from 38% to +36%.

JOURNAL OF HIGH ENERGY PHYSICS 5, 013, 2017. DOI: 10.1007/JHEP05(2017)013

[P103-2017] “Oscillatory behavior of light in the composite Goos-Hanchen shift”

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

For incidence in the critical region, the propagation of Gaussian lasers through dielectric blocks is characterized by the joint action of angular deviations and lateral displacements. This mixed effect, known as the composite Goos-Hanchen shift, produces a lateral displacement that is dependent on the axial coordinate, recently confirmed by a weak measurement experiment. We discuss under which conditions this axial lateral displacement, which only exists for the composite Goos-Hanchen shift, presents an oscillatory behavior. This oscillation phenomenon shows a peculiar behavior of light for critical incidence and, if experimentally tested, could stimulate further theoretical studies and lead to interesting optical applications.

PHYSICAL REVIEW A 95[5], 053836, 2017. DOI: 10.1103/PhysRevA.95.053836

[P104-2017] “ $\phi$ -Meson production at forward rapidity in

p-Pb collisions at  $\sqrt{s(NN)}=5.02$  TeV and in pp collisions at  $\sqrt{s}=2.76$  TeV”

Adam, J.; Adamova, D.; Aggarwal, M. M.; Chinellato, D. D.\*; Dash, A.\*; Takahashi, J.\*; et al. ALICE Collaboration

The first study of  $\phi$ -meson production in p-Pb collisions at forward and backward rapidity, at a nucleon-nucleon centre-of-mass energy  $\sqrt{s(NN)}=5.02$  TeV, has been performed with the ALICE apparatus at the LHC. The  $\phi$ -mesons have been identified in the dimuon decay channel in the transverse momentum ( $p(T)$ ) range  $1 < p(T) < 7$  GeV/c, both in the p-going ( $2.03 < y < 3.53$ ) and the Pb-going ( $-4.46 < y < -2.96$ ) directions - where  $y$  stands for the rapidity in the nucleon-nucleon centre-of-mass - the integrated luminosity amounting to 5.01  $\pm$  0.19 nb<sup>-1</sup> and 5.81  $\pm$  0.20 nb<sup>-1</sup>, respectively, for the two data samples. Differential cross sections as a function of transverse momentum and rapidity are presented. The forward-backward ratio for  $\phi$ -meson production is measured for  $2.96 < |y| < 3.53$ , resulting in a ratio similar to 0.5 with no significant  $p(T)$  dependence within the uncertainties. The  $p(T)$  dependence of the  $\phi$  nuclear modification factor  $R_{pPb}$  exhibits an enhancement up to a factor 1.6 at  $p(T) = 3-4$  GeV/c in the Pb-going direction. The  $p(T)$  dependence of the  $\phi$ -meson cross section in pp collisions at  $\sqrt{s} = 2.76$  TeV, which is used to determine a reference for the p-Pb results, is also presented here for  $1 < p(T) < 5$  GeV/c and  $2.5 < y < 4$ , for a 78  $\pm$  3 nb<sup>-1</sup> integrated luminosity sample.

PHYSICS LETTERS B 768, 203-217, 2017. DOI: 10.1016/j.physletb.2017.01.074

[P105-2017] “Photocatalytic oxidation of selected gas-phase VOCs using UV light, TiO<sub>2</sub>, and TiO<sub>2</sub>/Pd”

Fujimoto, T. M.; Ponczek, M.; Rochetto, U. L.; Landers, R.\*; Tomaz, E.

Heterogeneous photocatalytic oxidation systems using titanium dioxide (TiO<sub>2</sub>) have been extensively studied for the removal of several volatile organic compounds (VOCs). The addition of noble metals such as palladium on TiO<sub>2</sub> may improve photocatalytic activity by increasing charge separation efficiency. In this work, palladium was impregnated on TiO<sub>2</sub> and the efficiency of the new catalyst was tested and compared with that of pure TiO<sub>2</sub>. Pd was impregnated on TiO<sub>2</sub> by the reduction method, using NaBH<sub>4</sub>, and was characterized by XRD, XPS, UV-Vis, and H<sub>2</sub> chemisorption. The photocatalytic tests were performed in an annular coated-wall reactor using octane, isooctane, n-hexane, and cyclohexane at inlet concentrations varying from 100 to 120 ppmv. Compared with pure TiO<sub>2</sub> film, the photocatalytic activity of TiO<sub>2</sub> impregnated with 1 wt% of palladium was improved. All the aforementioned analytical techniques confirmed the presence of Pd incorporated into the structure of TiO<sub>2</sub>, and the conversion rates were studied in a broad range of residence times, yielding up to 90 % or higher rates in 40 s of residence time, thus underscoring the relevant contribution of the technology.

ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH 24[7], 6390-6396, 2017. DOI: 10.1007/s11356-016-6494-7

[P106-2017] “Radiography registration for mosaic tomography”

Vescovi, R. F. C.\*; Cardoso, M. B.; Miqueles, E. X.

A hybrid method of stitching X-ray computed tomography (CT) datasets is proposed and the feasibility to apply the scheme in a synchrotron tomography beamline with micrometre resolution is shown. The proposed method enables the field of view of the system to be extended while spatial resolution and experimental setup remain unchanged.



The approach relies on taking full tomographic datasets at different positions in a mosaic array and registering the frames using Fourier phase correlation and a residue-based correlation. To ensure correlation correctness, the limits for the shifts are determined from the experimental motor position readouts. The masked correlation image is then minimized to obtain the correct shift. The partial datasets are blended in the sinogram space to be compatible with common CT reconstructors. The feasibility to use the algorithm to blend the partial datasets in projection space is also shown, creating a new single dataset, and standard reconstruction algorithms are used to restore high-resolution slices even with a small number of projections.

**JOURNAL OF SYNCHROTRON RADIATION** 24, 686-694, 2017. DOI: 10.1107/S1600577517001953

**[P107-2017] “Relative Modification of Prompt  $\psi(2S)$  and  $J/\psi$  Yields from pp to PbPb Collisions at  $\sqrt{s}(NN)=5.02$  TeV”**

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

The relative modification of the prompt  $\psi(2S)$  and  $J/\psi$  yields from pp to PbPb collisions, at the center-of-mass energy of 5.02 TeV per nucleon pair, is presented. The analysis is based on pp and PbPb data samples collected by the CMS experiment at the LHC in 2015, corresponding to integrated luminosities of 28.0 pb<sup>-1</sup> and 464  $\mu$ b<sup>-1</sup>, respectively. The double ratio of measured yields of prompt charmonia reconstructed through their decays into muon pairs,  $(N(\psi(2S))/N(J/\psi))(PbPb)/(N(\psi(2S))/N(J/\psi))(pp)$ , is determined as a function of PbPb collision centrality and charmonium transverse momentum  $p_T$ , in two kinematic intervals: broken vertical bar  $y$  vertical bar < 1.6 covering  $6.5 < p_T < 30$  GeV/c and  $1.6 < \text{broken vertical bar } y \text{ vertical bar} < 2.4$  covering  $3 < p_T < 30$  GeV/c. The centrality-integrated double ratios are  $0.36 \pm 0.08(\text{stat}) \pm 0.05(\text{syst})$  in the first interval and  $0.24 \pm 0.22(\text{stat}) \pm 0.09(\text{syst})$  in the second. The double ratio is lower than unity in all the measured bins, suggesting that the  $\psi(2S)$  yield is more suppressed than the  $J/\psi$  yield in the explored phase space.

**PHYSICAL REVIEW LETTERS** 118[16], 162301, 2017. DOI: 10.1103/PhysRevLett.118.162301

**[P108-2017] “Search for electroweak production of a vector-like quark decaying to a top quark and a Higgs boson using boosted topologies in fully hadronic final states”**

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

A search is performed for electroweak production of a vector-like top quark partner  $T$  of charge  $2/3$  in association with a standard model top or bottom quark, using 2.3 fb<sup>-1</sup> of proton-proton collision data at TeV collected by the CMS experiment at the CERN LHC. The search targets  $T$  quarks decaying to a top quark and a Higgs boson in fully hadronic final states. For a  $T$  quark with mass above 1 TeV the daughter top quark and Higgs boson are highly Lorentz-boosted and can each appear as a single hadronic jet. Jet substructure and  $b$  tagging techniques are used to identify the top quark and Higgs boson jets, and to suppress the standard model backgrounds. An excess of events is searched for in the  $T$  quark candidate mass distribution in the data, which is found to be consistent with the expected backgrounds. Upper limits at 95% confidence level are set on the product of the single  $T$  quark production cross sections and the branching fraction, and these vary between 0.31 and 0.93 pb for  $T$  quark masses in the range 1000-1800 GeV. This is the first search for single electroweak production of a vector-like  $T$  quark in fully hadronic final states.

**JOURNAL OF HIGH ENERGY PHYSICS** 4, 136, 2017. DOI: 10.1007/JHEP04(2017)136

**[P109-2017] “Search for electroweak production of charginos in final states with two  $T$  leptons in pp collisions at  $\sqrt{s}=8$  TeV”**

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

Results are presented from a search for the electroweak production of supersymmetric particles in pp collisions in final states with two  $T$  leptons. The data sample corresponds to an integrated luminosity between 18.1 fb<sup>-1</sup> and 19.6 fb<sup>-1</sup> depending on the final state of  $T$  lepton decays, at  $\sqrt{s} = 8$  TeV, collected by the CMS experiment at the LHC. The observed event yields in the signal regions are consistent with the expected standard model backgrounds. The results are interpreted using simplified models describing the pair production and decays of charginos or  $T$  sleptons. For models describing the pair production of the lightest chargino, exclusion regions are obtained in the plane of chargino mass vs. neutralino mass under the following assumptions: the chargino decays into third-generation sleptons, which are taken to be the lightest sleptons, and the sleptons masses lie midway between those of the chargino and the neutralino. Chargino masses below 420 GeV are excluded at a 95% confidence level in the limit of a massless neutralino, and for neutralino masses up to 100 GeV, chargino masses up to 325 GeV are excluded at 95% confidence level. Constraints are also placed on the cross section for pair production of  $T$  sleptons as a function of mass, assuming a massless neutralino.

**JOURNAL OF HIGH ENERGY PHYSICS** 4, 018, 2017. DOI: 10.1007/JHEP04(2017)018

**[P110-2017] “Search for heavy resonances decaying into a vector boson and a Higgs boson in final states with charged leptons, neutrinos, and  $b$  quarks”**

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

A search for heavy resonances decaying to a Higgs boson and a vector boson is presented. The analysis is performed using data samples collected in 2015 by the CMS experiment at the LHC in proton-proton collisions at a center-of-mass energy of 13 TeV, corresponding to integrated luminosities of 2.2-2.5 fb<sup>-1</sup>. The search is performed in channels in which the vector boson decays into leptonic final states ( $Z \rightarrow \nu\nu$ ,  $W \rightarrow l\nu$ , and  $Z \rightarrow ll$ , with  $l = e, \mu$ ), while the Higgs boson decays to collimated  $b$  quark pairs detected as a single massive jet. The discriminating power of a jet mass requirement and a  $b$  jet tagging algorithm are exploited to suppress the standard model backgrounds. The event yields observed in data are consistent with the background expectation. In the context of a theoretical model with a heavy vector triplet, a resonance with mass less than 2 TeV is excluded at 95% confidence level. The results are also interpreted in terms of limits on the parameters of the model, improving on the reach of previous searches.

**PHYSICS LETTERS B** 768, 137-162, 2017. DOI: 10.1016/j.physletb.2017.02.040

**[P111-2017] “Search for massive resonances decaying in to  $WW, WZ$  or  $ZZ$  bosons 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

A search is presented for new massive resonances decaying to  $WW$ ,  $WZ$  or  $ZZ$  bosons in  $l$   $\bar{q}$  ( $q$ ) over  $\bar{q}$  ( $q$ ) over  $\bar{q}q$  ( $q$ ) over  $\bar{q}$  final states. Results are based on data corresponding to an integrated luminosity of  $2.3$ - $2.7$   $\text{fb}^{-1}$  recorded in proton-proton collisions at  $\sqrt{s} = 13$  TeV with the CMS detector at the LHC. Decays of spin-1 and spin-2 resonances into two vector bosons are sought in the mass range  $0.6$ - $4.0$  TeV. No significant excess over the standard model background is observed. Combining the results of the  $l$   $\bar{q}$  ( $q$ ) over  $\bar{q}$  and  $q$  ( $q$ ) over  $\bar{q}q$  ( $q$ ) over  $\bar{q}$  final states, cross section and mass exclusion limits are set for models that predict heavy spin-1 and spin-2 resonances. This is the first search for a narrow-width spin-2 resonance at  $\sqrt{s} = 13$  TeV.

**JOURNAL OF HIGH ENERGY PHYSICS 3, 162, 2017. DOI: 10.1007/JHEP03(2017)162**

**[P112-2017] “Search for narrow resonances in dilepton mass spectra in proton-proton collisions at  $\sqrt{s}=13$  TeV and combination with 8 TeV data”**

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

A search for narrow resonances in dielectron and dimuon invariant mass spectra has been performed using data obtained from proton-proton collisions at  $\sqrt{s} = 13$  TeV collected with the CMS detector. The integrated luminosity for the dielectron sample is  $2.7$   $\text{fb}^{-1}$  and for the dimuon sample  $2.9$   $\text{fb}^{-1}$ . The sensitivity of the search is increased by combining these data with a previously analyzed set of data obtained at  $\sqrt{s} = 8$  TeV and corresponding to a luminosity of  $20$   $\text{fb}^{-1}$ . No evidence for non-standard-model physics is found, either in the 13 TeV data set alone, or in the combined data set. Upper limits on the product of production cross section and branching fraction have also been calculated in a model-independent manner to enable interpretation in models predicting a narrow dielectron or dimuon resonance structure. Limits are set on the masses of hypothetical particles that could appear in new-physics scenarios. For the  $Z'$  (SSM) particle, which arises in the sequential standard model, and for the superstring inspired  $Z'$  ( $\psi$ ) particle, 95% confidence level lower mass limits for the combined data sets and combined channels are found to be  $3.37$  and  $2.82$  TeV, respectively. The corresponding limits for the lightest Kaluza-Klein graviton arising in the Randall-Sundrum model of extra dimensions with coupling parameters  $0.01$  and  $0.10$  are  $1.46$  and  $3.11$  TeV, respectively. These results significantly exceed the limits based on the 8 TeV LHC data.

**PHYSICS LETTERS B 768, 57-80, 2017. DOI: 10.1016/j.physletb.2017.02.010**

**[P113-2017] “Search for R-parity violating supersymmetry with displaced vertices in proton-proton collisions at  $\sqrt{s}=8$  TeV”**

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

Results are reported from a search for R-parity violating supersymmetry in proton-proton collision events collected by the CMS experiment at a center-of-mass energy of  $\sqrt{s} = 8$  TeV. The data sample corresponds to an integrated luminosity of  $17.6$   $\text{fb}^{-1}$ . This search assumes a minimal flavor violating model in which the lightest supersymmetric particle is a long-lived neutralino or gluino, leading to a signal with jets emanating from displaced vertices. In a sample of events with two displaced vertices,

no excess yield above the expectation from standard model processes is observed, and limits are placed on the pair production cross section as a function of mass and lifetime of the neutralino or gluino. At 95% confidence level, the analysis excludes cross sections above approximately  $1$  fb for neutralinos or gluinos with mass between  $400$  and  $1500$  GeV and mean proper decay length between  $1$  and  $30$  mm. Gluino masses are excluded below  $1$  and  $1.3$  TeV for mean proper decay lengths of  $300$   $\mu\text{m}$  and  $1$  mm, respectively, and below  $1.4$  TeV for the range  $2$ - $30$  mm. The results are also applicable to other models in which long-lived particles decay into multijet final states.

**PHYSICAL REVIEW D 95[1], 012009, 2017. DOI: 10.1103/PhysRevD.95.012009**

**[P114-2017] “Search for supersymmetry in events with one lepton and multiple jets in proton-proton collisions at  $\sqrt{s}=13$  TeV”**

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

A search for supersymmetry is performed in events with a single electron or muon in proton-proton collisions at a center-of-mass energy of  $13$  TeV. The data were recorded by the CMS experiment at the LHC and correspond to an integrated luminosity of  $2.3$   $\text{fb}^{-1}$ . Several exclusive search regions are defined based on the number of jets and b-tagged jets, the scalar sum of the jet transverse momenta, and the scalar sum of the missing transverse momentum and the transverse momentum of the lepton. The observed event yields in data are consistent with the expected backgrounds from standard model processes. The results are interpreted using two simplified models of supersymmetric particle spectra, both of which describe gluino pair production. In the first model, each gluino decays via a three-body process to top quarks and a neutralino, which is associated with the observed missing transverse momentum in the event. Gluinos with masses up to  $1.6$  TeV are excluded for neutralino masses below  $600$  GeV. In the second model, each gluino decays via a three-body process to two light quarks and a chargino, which subsequently decays to a W boson and a neutralino. The mass of the chargino is taken to be midway between the gluino and neutralino masses. In this model, gluinos with masses below  $1.4$  TeV are excluded for neutralino masses below  $700$  GeV.

**PHYSICAL REVIEW D 95[1], 012011, 2017. DOI: 10.1103/PhysRevD.95.012011**

**[P115-2017] “Staggered quantum walks with Hamiltonians”**

Portugal, R.; de Oliveira, M. C.\*; Moqadam, J. K.\*

Quantum walks are recognizably useful for the development of new quantum algorithms, as well as for the investigation of several physical phenomena in quantum systems. Actual implementations of quantum walks face technological difficulties similar to the ones for quantum computers, though. Therefore, there is a strong motivation to develop new quantum-walk models which might be easier to implement. In this work we present an extension of the staggered quantum walk model that is fitted for physical implementations in terms of time-independent Hamiltonians. We demonstrate that this class of quantum walk includes the entire class of staggered quantum walk model, Szegedy's model, and an important subset of the coined model.

**PHYSICAL REVIEW A 95[1], 012328, 2017. DOI: 10.1103/PhysRevA.95.012328**

**[P116-2017] “Staggered quantum walks with superconducting microwave resonators”**

Moqadam, J. K.\*; de Oliveira, M. C.\*; Portugal, R.

The staggered quantum walk is a model defined by the product of local operators associated with two or more independent graph tessellations. This model is versatile, encompasses several well-known discrete-time quantum walks, and inherits interesting features of the continuous-time quantum walk. We propose an implementation of the staggered quantum walk model with superconducting microwave resonators, where the required local operations are provided by the nearest neighbor interaction of the resonators coupled through superconducting quantum interference devices. The tunability of the interactions makes this system an excellent toolbox for this class of quantum walks. We focus on the one-dimensional case and discuss its generalization to a more general class known as triangle-free graphs.

PHYSICAL REVIEW B 95[14], 144506, 2017. DOI: 10.1103/PhysRevB.95.144506

[P117-2017] “Structural and magnetic phase transition observed in the YCrO<sub>3</sub>+ $\gamma$  compound”

Fabian, F. A.; Moura, K. O.\*; Barbosa, C. C. S.; Peixoto, E. B.; Garcia, F.; Duque, J. G. S.\*; Meneses, C. T.

We report on thermogravimetric, structural and magnetization measurements in the YCrO<sub>3</sub>+ $\gamma$  compound obtained by the co-precipitation method. The thermogravimetric analyses show that the weight losses which occur at three distinct steps are associated with water evaporation, formation of zircon-type YCrO<sub>4</sub> compound and finally a phase transition from the tetragonal YCrO<sub>4</sub> to the orthorhombic YCrO<sub>3</sub>. The X-ray diffraction measurements allied with the Rietveld refinement confirm such trend, that is, the observed X-ray patterns are consistent with a gradual growth of zircon-type YCrO<sub>4</sub> with tetragonal structure and space group I4<sub>1</sub>/amd for annealing temperatures up to 600 degrees C followed by the phase transition to the orthorhombic YCrO<sub>3</sub> phase with space group Pbnm for annealing temperatures above 625 degrees C. The X-ray absorption near edge structure (XANES) spectra carried out in the Cr K-edge reveal that the oxidation states of Cr ions depend on the synthesis temperature. The T-dependencies of magnetic susceptibility point out a ferromagnetic-antiferromagnetic transition as function synthesis temperature. The Curie and Neel temperatures are in agreement with that reported in literature for the YCrO<sub>4</sub> and YCrO<sub>3</sub> compounds, respectively. Besides, the MvsH curves measured at 2 and 50 K are consistent with the observed magnetic states to each sample.

JOURNAL OF ALLOYS AND COMPOUNDS 702, 244-248, 2017. DOI: 10.1016/j.jallcom.2016.12378

[P118-2017] “Structural Reinforcement through Liquid Encapsulation”

Chipara, A. C.; Owuor, P. S.; Bhowmick, S.; Brunetto, G.; Asif, S. A. S.; Chipara, M.; Vajtai, R.; Lou, J.; Galvao, D. S.\*; Tiwary, C. S.; Ajayan, P. M.

The liquid inside a solid material is one of the most common composite materials in nature. The interface between solid-liquid plays an important role in unique deformation. Here, model systems of two polymers (polydimethylsiloxane-polyvinylidene-fluoride) are used to make sphere of solid with liquid inside it.

ADVANCED MATERIALS INTERFACES 4[2], 1600781, 2017. DOI: 10.1002/admi.201600781

[P119-2017] “Suppression and azimuthal anisotropy of prompt and nonprompt J/psi production in PbPb collisions at root S-NN=2.76 TeV”

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

CMS Collaboration

The nuclear modification factor R-AA and the azimuthal anisotropy coefficient v(2) of prompt and nonprompt (i.e. those from decays of b hadrons) J/psi mesons, measured from PbPb and pp collisions at root S-NN = 2.76 rfeV at the LHC, are reported. The results are presented in several event centrality intervals and several kinematic regions, for transverse momenta p(T) > 6.5 GeV/c and rapidity vertical bar y vertical bar < 2.4, extending down to p(T) = 3 GeV/c in the 1.6 < vertical bar y vertical bar < 2.4 range. The v(2) of prompt J/psi is found to be nonzero, but with no strong dependence on centrality, rapidity, or p(T) over the full kinematic range studied. The measured v(2) of nonprompt J/psi is consistent with zero. The R-AA of prompt J/psi exhibits a suppression that increases from peripheral to central collisions but does not vary strongly as a function of either y or pT in the fiducial range. The non-prompt J/psi RAA shows a suppression which becomes stronger as rapidity or p(T) increases. The v(2) and R-AA of open and hidden charm, and of open charm and beauty, are compared.

EUROPEAN PHYSICAL JOURNAL C 77[4], 252, 2017. DOI: 10.1140/epjc/s10052-017-4781-1

[P120-2017] “Surface Propensity of Atmospherically Relevant Amino Acids Studied by XPS”

Mocellin, A.; de Abreu Gomes, A. H.\*; Araujo, O. C.; de Brito, A. N.\*; Bjorneholm, O.

Amino acids constitute an important fraction of the water-soluble organic nitrogen (WSON) compounds in aerosols and are involved in many processes in the atmosphere. In this work, we applied X-ray photoelectron spectroscopy (XPS) to study aqueous solutions of four amino acids, glycine, alanine, Valine, and methionine, in their zwitterionic forms. We found that amino acids with hydrophilic side chains and smaller size, GLY and ALA, tend to stay in the bulk of the liquid, while the hydrophobic and bigger amino acids, VAL and MET, are found to concentrate more on the surface. We found experimental evidence that the amino acids have preferential orientation relative to the surface, with the hydrophobic side chain being closer to the surface than the hydrophilic carboxylate group. The observed amino acid surface propensity has implications in atmospheric science as the surface interactions play a central role in cloud droplet formation, and they should be considered in climate models.

JOURNAL OF PHYSICAL CHEMISTRY B 121[16], 4220-4225, 2017. DOI: 10.1021/acs.jpcc.7b02174

[P121-2017] “Training-induced inversion of spontaneous exchange bias field on La<sub>1.5</sub>Ca<sub>0.5</sub>CoMnO<sub>6</sub>”

Bufaical, L.; Finkler, R.; Coutrim, L. T.; Pagliuso, P. G.\*; Grossi, C.; Stavale, F.; Baggio-Saitovitch, E.; Bittar, E. M.

In this work we report the synthesis and structural, electronic and magnetic properties of La<sub>1.5</sub>Ca<sub>0.5</sub>CoMnO<sub>6</sub> double-perovskite. This is a re-entrant spin cluster material which exhibits a non-negligible negative exchange bias effect when it is cooled in zero magnetic field from an unmagnetized state down to low temperature. X-ray powder diffraction, X-ray photoelectron spectroscopy and magnetometry results indicate mixed valence state at Co site, leading to competing magnetic phases and uncompensated spins at the magnetic interfaces. We compare the results for this Ca-doped material with those reported for the resembling compound La<sub>1.5</sub>Sr<sub>0.5</sub>CoMnO<sub>6</sub>, and discuss the much smaller spontaneous exchange bias effect observed for the former in terms of its structural and magnetic particularities.



For La<sub>1.5</sub>Ca<sub>0.5</sub>CoMnO<sub>6</sub>, when successive magnetization loops are carried, the spontaneous exchange bias field inverts its sign from negative to positive from the first to the second measurement. We discuss this behavior based on the disorder at the magnetic interfaces, related to the presence of a glassy phase. This compound also exhibits a large conventional exchange bias, for which there is no sign inversion of the exchange bias field for consecutive cycles.

**JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS 433, 271-277, 2017. DOI: 10.1016/j.jmmm.2017.03.017**

**[P122-2017] “Transient negative ion spectrum of the cytosine-guanine pair”**

Nunes, F. B.; Varella, M. T. N.; Pastega, D. F.; Freitas, T. C.; Lima, M. A. P.\*; Bettega, M. H. F.; Sanchez, S. D.

We employed elastic scattering calculations, performed in the static exchange approximation, to investigate the  $\pi^*$  anion states of cytosine, guanine and the cytosine-guanine pair. Our results for the isolated monomers, also obtained in the static-exchange plus polarization approximation, are in good agreement with the available calculations and electron transmission data. Virtual orbital analysis for the lower-lying  $\pi^*$  anion states, with pure shape resonance character, indicates that electron attachment to the cytosine-guanine pair gives rise to resonances located on either monomer (the orbitals do not delocalize over the pair). The  $\pi^*$  shape resonances of the pair localized on the cytosine unit have lower energies in comparison with those of the isolated base, with the opposite trend for the guanine unit. The underlying mechanism would be the net positive charge transfer to the cytosine unit, as the guanine monomer acts as a proton donor in two out of the three hydrogen bonds formed in the pair. Even though the calculations were performed in the static-exchange approximation (due to the size of the system), the conclusions drawn were also corroborated by empirical estimates of the vertical attachment energies. The results for the cytosine-guanine pair are compared to those previously obtained for the formic acid-formamide complex, having two hydrogen bonds with opposite donor/acceptor characters and negligible charge transfer.

**EUROPEAN PHYSICAL JOURNAL D 71[4], 92, 2017. DOI: 10.1140/epjd/e2017-70786-5**

**[P123-2017] “X-ray powder diffraction of high-absorption materials at the XRD1 beamline off the best conditions: Application to (Gd, Nd)(5)Si-4 compounds”**

Carvalho, A. M. G.; Nunes, R. S.; Coelho, A. A.\*

Representative compounds of the new family of magnetic materials Gd<sub>5-x</sub>Nd<sub>x</sub>Si<sub>4</sub> were analyzed by X-ray diffraction at the XRD1 beamline at Laboratorio Nacional de Luz Síncrotron. To reduce X-ray absorption, thin layers of the powder samples were mounted outside the capillaries and measured in Debye-Scherrer geometry as usual. The XRD analyses and the magnetometry results indicate that the behavior of the magnetic transition temperature as a function of Nd content may be directly related to the average of the four smallest interatomic distances between different rare earth sites of the majority phase of each compound. The quality and consistency of the results show that the XRD1 beamline is able to perform satisfactory XRD experiments on high-absorption materials even off the best conditions.

**POWDER DIFFRACTION 32[1], 10-14, 2017. DOI: 10.1017/S0885715616000646**

## Eventos publicados

**[P124-2017] “Identified particle production in pp collisions at  $\sqrt{s}=7$  and 13 TeV measured with ALICE”**

de Souza, R. D.\*; ALICE Collaboration  
Huang, H. Z.; Seto, R.; Thader, J.; Xu, N. (Ed.)

Proton-proton (pp) collisions have been used extensively as a reference for the study of interactions of larger colliding systems at the LHC. Recent measurements performed in high-multiplicity pp and proton-lead (p-Pb) collisions have shown features that are reminiscent of those observed in lead-lead (Pb-Pb) collisions. In this context, the study of identified particle spectra and yields as a function of multiplicity is a key tool for the understanding of similarities and differences between small and large systems. We report on the production of pions, kaons, protons,  $K_S^0$ ,  $\Lambda$ ,  $\Xi$ ,  $\Omega$  and  $K^*0$  as a function of multiplicity in pp collisions at  $\sqrt{s} = 7$  TeV measured with the ALICE experiment. The work presented here represents the most comprehensive set of results on identified particle production in pp collisions at the LHC. Spectral shapes, studied both for individual particles and via particle ratios as a function of PT, exhibit an evolution with charged particle multiplicity that is similar to the one observed in larger systems. In addition, results on the production of light flavour hadrons in pp collisions at  $\sqrt{s} = 13$  TeV, the highest centre-of-mass energy ever reached in the laboratory, are also presented and compared with previous, lower energy results.

**16TH INTERNATIONAL CONFERENCE ON STRANGENESS IN QUARK MATTER (SQM2016), Univ Calif, Clark Kerr Campus, Berkeley, CA. JUN 27-JUL 01, 2016.  
Journal of Physics Conference Series 779, UNSP 012071, 2017. DOI:10.1088/1742-6596/779/1/012071**

**[P125-2017] “Sensitivity of a PMMA polymer capillary microresonator for measuring relative humidity”**

Padilla, D. A. A.; Moreno, C. T.; Cristiano M. B. C.\*  
IOP

This paper studied experimentally the behavior of a capillary microresonator made from PMMA polymer as a sensor for measuring relative humidity. In the manufactured device, the WGMS modes within the microcavity are excited by the proximity of an optical fiber Taper made from the stretching of a standard optical fiber of silica by the method of scanning flame with waist of the order of 3-5  $\mu$ m. In the device, the field from a tunable laser system TLS is coupled into the capillary along its cross section where the resonant modes were observed WGMS into the cavity. When the system is subjected to change of the relative humidity of the external environment, the wavelengths of peaks resonances of WGMS modes of the resonant system experience a spectral shift, so that a sensitivity of the microresonator is observed at changes in humidity of the external environment. During the experiment, it was manufactured capillaries with different diameters and different wall thickness obtaining a sensitivity of the order of 0.07 nm/% RH for a capillary thickness 42.1  $\mu$ m.

**VIII INTERNATIONAL CONGRESS OF ENGINEERING PHYSICS, Merida, MEXICO. NOV 07-11, 2016.  
Journal of Physics Conference Series 792, UNSP, 012050, 2017. DOI: 10.1088/1742-6596/792/1/012050**

## Artigos aceitos para publicação

[A001-2017] “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: <https://doi.org/10.1016/j.diamond.2017.06.002>

Received 5 April 2017, Revised 5 May 2017, Accepted 7 June 2017, Available online 8 June 2017.

\*Autores da comunidade IFGW

Fonte: Web of Science on-line.

## Defesas de Dissertações

[D002-2017] “Teoria Quântica de Campos em Referenciais Acelerados”

Aluno: Henrique Dias Truran

Orientador: Prof. Dr. Donato Giorgio Torrieri

Data: 28/06/2017

[D003-2017] “Revelando a estrutura eletrônica de nanomateriais através de espectroscopia óptica avançada”

Aluno: Gabriel Nagamine

Orientador: Prof. Dr. Lázaro Aurélio Padilha Júnior

Data: 29/06/2017

[D004-2017] “Estudos de ressonância de spin eletrônico (RSE) em isolantes topológicos dopados com terras-raras”

Aluno: Jean Carlo Souza

Orientador: Prof. Dr. Pascoal José Giglio Pagliuso

Data: 30/06/2017

[D005-2017] “Síntese e caracterização de monocristais de Sr<sub>1-x</sub>EuxFe<sub>2</sub>As<sub>2</sub> preparados pelo método do fluxo de In”

Aluno: Matheus Radaelli

Orientador: Prof. Dr. Pascoal José Giglio Pagliuso

Data: 07/07/2017

## Defesas de Teses

[T009-2017] “Dosimetria in vitro em BNCT com o uso de filmes finos de boro e detectores PADC”

Aluno: Bárbara Smilgys

Orientador: Prof. Dr. Sandro Guedes de Oliveira

Data: 26/05/2017

[T010-2017] “Crescimento de nanofios via o método de nanonucleação por fluxo metálico: Explorando efeitos da dimensionalidade nas interações magnéticas fundamentais”

Aluno: Karoline Oliveira Moura

Orientador: Prof. Dr. Kleber Roberto

Data: 26/05/2017

[T011-2017] “Estudo de Processos de Adesão Bacteriana: Propriedades Mecânicas e Efeitos do Microambiente Sobre Adesão, Crescimento e Mobilidade da Xylella Fastidiosa”

Aluno: Moniellen Pires Monteiro

Orientador: Profa. Dra. Mônica A. Cotta

Data: 06/06/2017

[T012-2017] “Optomecânica de cavidades em discos de silício e discos nanoestruturados de silício”

Aluno: Felipe Gustavo da Silva Santos

Orientador: Prof. Dr. Thiago Pedro Mayer Alegre

Data: 09/06/2017

**[T013-2017] “Fenômenos Quânticos e Localização em Sistemas Optomecânicos”**

Aluno: Thales Figueiredo Roque

Orientador: Prof. Dr. Antonio Vidiella Barranco

Data: 21/06/2017

**[T014-2017] “Estudo da dinâmica de sistemas da matéria condensada por difração de raios X resolvida no tempo”**

Aluno: Kelin Regina Tasca

Orientador: Profa. Dra. Cris Adriano

Data: 22/06/2017

**[T015-2017] “Fibras Ópticas Especiais para Sensoriamento”**

Aluno: Jonas Henrique Osório

Orientador: Prof. Dr. Cristiano Monteiro de Barros Cordeiro

Data: 12/07/2017

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

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

O **Abstracta** é um boletim bimestral destinado à divulgação da produção científica da comunidade do Instituto de Física “Gleb Wataghin” - IFGW da Universidade Estadual de Campinas - Unicamp.

**Fique por dentro!**

Cadastre-se como leitor, e receba aviso da publicação de novos números por e-mail:

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

## Abstracta

Instituto de Física

Diretor: Prof. Dr. Newton Cesario Frateschi

Diretor Associado: Prof. Dr. Luís Eduardo

Evangelista de Araujo

Universidade Estadual de Campinas - UNICAMP

Cidade Universitária Zeferino Vaz

13083-859 - Campinas - SP - Brasil

e-mail: [secdir@ifi.unicamp.br](mailto:secdir@ifi.unicamp.br)

## Publicação

Biblioteca do Instituto de Física Gleb Wataghin  
<http://portal.ifi.unicamp.br/biblioteca>

Diretora Técnica: Sandra Maria Carlos Cartaxo  
Coordenador da Comissão de Biblioteca: Prof. Dr. André Koch Torres de Assis

Elaboração

Maria Graciele Trevisan (Bibliotecária)

Ayres Neri da Cunha Junior

contato: [infobif@ifi.unicamp.br](mailto:infobif@ifi.unicamp.br)