

# FÍSICA 2022

23<sup>a</sup> Conferência  
Nacional de Física

32<sup>o</sup> Encontro Ibérico  
para o Ensino da Física

7—10  
Setembro,  
2022

Física do Clima

Gravitação

Grafeno & “ângulo mágico”

Eletrónica Flexível

100 anos da experiência  
de Stern-Gerlach

Faculdade de  
Ciências da  
Universidade  
do Porto

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## Início

A **FÍSICA 2022 – 23ª Conferência Nacional de Física e 32º Encontro Ibérico para o Ensino da Física**, realiza-se na Faculdade de Ciências da Universidade do Porto de 7 a 10 de Setembro de 2022, em regime presencial.

Esta conferência bienal, organizada pela Sociedade Portuguesa de Física reúne toda a comunidade nacional de físicos, abrangendo docentes do Ensino Básico ao Superior, Investigadores e Estudantes de todas as áreas da Física, numa partilha do estado atual do conhecimento em Física.

A **FÍSICA 2022** terá sessões plenárias, sessões paralelas e pósteres nas áreas de todas as suas Divisões Científicas:

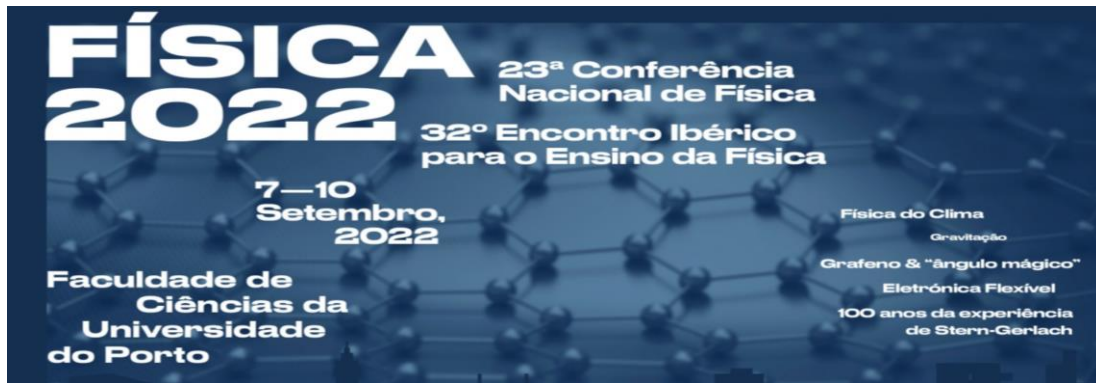
Astronomia e Astrofísica, Educação, Física Aplicada à Engenharia e em Empresa, Física Atómica e Molecular, Física da Matéria Condensada, Física Médica, Física Nuclear, Física das Partículas, Física dos Plasmas, Geofísica, Oceanografia e Meteorologia, História da Física, Óptica e Lasers.

Na Física 2022 daremos relevo em duas Plenárias aos temas dos prémios Nobel de Física de 2020 e 2021.

- **buracos negros**
- **compreensão de sistemas complexos**

O 32º Encontro Ibérico para o Ensino da Física organizado este ano em colaboração com a Real Sociedad Española de Física e o Instituto de Educação da UL será um momento de formação para os professores do ensino básico, secundário e superior. Pretende-se ainda sensibilizar os governantes para a necessidade da renovação dos quadros de docência no Ensino Básico, Secundário e Superior e os desafios que este rejuvenescimento coloca à formação académica.

O Encontro Ibérico está acreditado como Ação de Formação de 25 horas.



### Local

Faculdade de Ciências da Universidade do Porto

Departamento de Ciências de Computadores - FC6

Rua Campo Alegre 1021/1055

4169-007 Porto

Auditório Ferreira da Silva





8 setembro Quinta-feira			
Anfiteatro 029	Sala 140	Anfiteatro 030	
Matéria Condensada	Física Nuclear	Ensino da Física	
14:30	Theory of the Nonlinear Optical Conductivity/ D J Passos		Distinguished Scientists: From Creativity to Knowledge/ Maria Matilde Ariza Montes
14:45	Bose-Einstein Condensates in Quasi-periodic Lattices: Bosonic Josephson Junction and Multi-mode Dynamics/ H Prates	INVITED: Patricia Gonçalves (Titulo a ser divulgado)	Proteção dos Olhos Contra a Radiação Ultravioleta/ Luis Filipe Pereira Franco Afonso
15:00	Dielectric And Magnetic Properties of Ca3Mn2O7 Thin Films/ Bruna Silva		Holographic Optical Instruments Production and Holographic Interferometry as Contents for Laboratory Practices for Undergraduate Students in Physics and Physics Teaching/ José Caiongo Chibaca
15:15	Structural and Magnetic Transformations Induced by Mn Doping in Ca- and Sr- substituted BiFeO3/ M Das	Analysis of Gan Core-Shell P-N Junction Nanowire Radiation Detectors Irrac	Programa de Simulação de Queda em Fluidos/ Rui J. Agostinho e Ana Tavares Sousa
15:30	Shape Transition of Sedimenting Confined Capsules/ Danilo Silva	Cr-doped $\beta$ -Ga2O3: Luminescence Activation by Irradiation-Induced Defects	Spins Primeiro, Para Não Ficar Para Trás/ Vítor Brás de Sequeira Amaral
15:45	The role of Structural Distortions in Triggering the Metal to Insulator Transition in NdNiO3/ M M Gomes		Capacidades Térmicas: Aspectos Teóricos e Didáticos/ Joaquim Manuel da Silva Anacleto
16:00	Density Functional Theory and Perturbed Angular Correlation Study of the AMnGe2O6 (A=Be, Mg, Ca, Sr) Clinopyroxene Series/ R Moreira	INVITED: Renân Pereira (Titulo a ser divulgado)	Calor e Trabalho: Equívocos e Soluções/ Joaquim Manuel da Silva Anacleto
16:15	Percolation Based Simulation to Predict Caking Kinetics of Polydispersed Amorphous Powders/ V Braz		A Ciência por Detrás dum Pêndulo: indo além do Pêndulo Físico / Horácio Fernandes

8 setembro Quinta-feira			
Anfiteatro 029	Sala 140	Anfiteatro 030	
Óptica e Lasers	Física Médica e para a Ciência da Vida	Geofísica, Oceanografia e Meteorologia	
17:30	Optical Tweezers Development as a Tool for Biomedical Diagnosis/J. Freitas Oliveira		Climate in the Eastern Boundary of the Atlantic/Pedro Manuel Alberto De Miranda
17:45	Optical Properties of One-Dimensional Periodic Structures: From Photonic Crystals to Hyperbolic Metamaterials/Bernardo Dias	INVITED: Membrane biophysics: a meeting point for new therapies / Claudia Nunes	Potencial Migração da Adequação Bioclimática de Diferentes Castas de Uva Portuguesas na Europa Devido às Alterações Climáticas/Filipe Jorge Santos Ferreira Adão
18:00	Optical Fiber Sensor For Measuring Water Vapour Sorption Hysteresis of Cement Paste/P. M. Da Silva		Assessing the Future Wind Energy Potential Along the Portuguese Coast Using Cmp6 Model Ensemble and WRT High Resolution Simulations/ André Filipe Monteiro Claro
18:15	Development of a Biogenic Amine Optic Sensor Using Rosamine in a Cellulose Membrane /Simão Seixas	Revestimentos funcionais para aplicações óticas e oftálmicas / Silvana Guedes	Biases in the Variability of the Vertically Averaged Atmospheric Circulation Simulated by Cmp6 Models/ José Manuel Castanheira
18:30	Development of an Optical Magnetic Field Sensor Based on Surface Plasmon Resonance and Magnetostriction/ João P. M. Carvalho	Surface functionalization of spin-vortex nano-discs for magneto-mechanically induced damage applications / Ricardo Magalhaes	Lightning Modelling In Numerical Weather Prediction /Rui Salgado
18:45	Development of Optical Gas Sensors Based on Porous Materials/ Mariana A. F. De Melo E Sousa	Hemodinâmica Na Bifurcação Da Artéria Aorta Abdominal Com Um Modelo De Duas Fases / Daniela O. Trigo	Modelling Atmospheric Conditions Leading To Large Fires In Portugal/Cátia Isabel Nunes Campos
19:00	Nanostructures Towards Near Infrared Sensing/ Paulo S. S. Dos Santos	Wound Opening In A Thin Incompressible Viscoelastic Tissue / G. M. Carvalho	Measurements Of Evaporation In Mediterranean And Antarctica Lakes/Miguel Joaquim Fernandes Potes
19:15	Mineral Identification Using Laser Induced Breakdown Spectroscopy Mapping / Diana Capela	Volumetric Interferometric Lattice Light-Sheet Imaging / Simão Coelho	Dinamic And Diabatic Processes In Extratropical Cy-Clones In The Atlantic Region/ Margarida L. R. Liberato
19:30			Observed Geomagnetic Field Anomalies and Possible Consequences / Maria Rosa Duque

Sexta-feira, 9 setembro			
Anfiteatro 029	Sala 140	Anfiteatro 030	
Óptica e Lasers	Física Médica e para a Ciência da Vida	Ensino da Física	
14:30	Development and Characterization of an Ultra-Broadband 7 Fs Laser Oscillator For Multicolor Nonlinear Imaging / Tiago E. C. Magalhães		Adição de Elementos Multimédia em Applets de Física Para Alunos Com Dislexia/ Léo Rodrigues Macena Dos Santos
14:45	Temporal Characterization Of Broadband Femtosecond Laser Pulses By Surface Third-Harmonic Dispersion Scan With Ptychographic Retrieval/Tiago Gomes	INVITED: Multifunctional lipid nanoparticles as a promising therapeutic strategy for breast cancer: Andreia Granja	Astronomy Projects at School: Interdisciplinarity In Science Teaching/ Álvaro Manuel Folhas Ferreira
15:00	Thz Time-Domain Spectroscopy Using A Femtosecond Laser-Plasma Source/Ana Oliveira E Silva		Projeto Viab-Fis: Uma Proposta Prático-Laboratorial Inclusiva para o Ensino Secundário/ Natália Alves Machado
15:15	Taming Light For Novel Computing Machines/Duarte Silva	Resistive-Switching Device Based On A Copper Solution For Artificial Synapses / Andreia Silva,	Physics Activities Developed in the Project Fisastee/ José António Araújo Gonçalves
15:30	Using Fluids Of Light In Photorefractive Media To Create Turbulent States/Tiago D. Ferreira	Overview Of Mpgd Based Full-Field Imaging Spectrometers – Current Status, Applications, And Future Directions / P. M. S. Carvalho	Atividades Experimentais Virtuais no Ensino Experimental da Física/ Marcelo José Rodrigues
15:45	Modelling the Final Electron Spectra After Radiation Reaction From Intense Laser Scattering/Oscar Amaro	Simulação Do Transporte Da Lipoproteína De Baixa Densidade Na Artéria Aorta Abdominal / Eliana M. Seixas	Como Organizar o Ensino Experimental de Física na Pós-Pandemia?/ José Jorge Da Silva Teixeira
16:00	Ultrafast Optical Pump-Probe Spectroscopy System for the Study of Photophysical Processes in Nanomaterials/Tânia M. Ribeiro	Applying Machine Learning Techniques For Quality Evaluation Of Complex Radiotherapy Treatments / B. Mendes	Capoeiras Jogam Física?! Um Exemplo da Introdução da Cultura de Matriz Africana na Física Escolar/ Wagner De Souza
16:15	Ultrafast Magnetization Dynamics in Cofeb-Based Multilayer Thin Films Down to the Few-Cycle Regime/Ana S. Silva	MCDHF Calculations Of Emission Rates In Radionuclides With Biomedical Interest / José M. P. Marques	

Sexta-feira, 9 setembro			
Anfiteatro 029	Sala 140	Anfiteatro 030	
Astrofísica, Cosmologia, Física de Altas Energias	Física dos Plasmas	Energia e Física Aplicada	
17:30	Parametric Design of a Cross Dispersed Echelle Spectrograph With Off-The-Shelf Components/ Nuno Cabecinhas Gonçalves	INVITED: Plasmas Contendo CO2: das Energias Renováveis às Atmosferas Planetárias/Carlos Daniel Pintassilgo	Anode-Less Secondary Lithium Battery/ Manuela Carvalho Baptista
17:45	Stellar Characterization for the ARIEL Space Mission/ Andreas Silva Neitzel		Capacitive Effect in Rechargeable Sodium Seawater/ João Ferreira
18:00	Deep Learning in Stellar Detection and Photometry/ Miguel Costa e Silva	INVITED: Energia a fusão nuclear com campos magnéticos 3D: tokamaks vs stellarators / Rogério Jorge	Energy Harvesting and Storage Textile-Based Device/ Rui Costa
18:15	The Gravity Experiment and the 2020 Physics Nobel Prize/ Paulo Valente Garcia		Improving Hematite Performance for Green Hydrogen/ João Freitas
18:30	Gravity: The Dark Side of the Force/ Cláudio Vieira Gomes	Simulating Fast Particle Confinement for New Stellarator Configurations/ Clara Cottet	Magnetic Tunnel Junctions Embeded with Paramagnetic Centers for Energy Harvesting/ Maria Gracio
18:45	Large Scale Atomic Structure Calculations in Kilonovae Modeling/ Jorge Almeida Sampaio	Plasma Physics Education Using ZPIC/ Miguel Pardal	Increase the Performance of the Thermoelectric Generator Thought Printed Collectors/ Ana Pires
19:00	Pentaquarks in a Bethe Salpeter Approach/ Luis Torres Rojas	Modelling a Hollow Cathode Discharge for Several Noble Gases/ Eduardo Calvo	Energy Harvesting Combining Thermomagnetic Materials and Triboelectric Nanogenerators/ Rita Bugalhão
19:15	Heavy Baryon Spectroscopy in a Quark-Diquark Approach/ André Torcato		Magsense/ Gabriel Dinis
19:30	Going to the Light-Front with Contour Deformations/ Eduardo Bento Ferreira		Correntes Geomagneticamente Induzidas Agregam Indústria E Ciência / Rute Rodrigues Santos



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## Plenárias

# Os ângulos mágicos do Carbono

João Lopes dos Santos

Departamento de Física e Astronomia da Faculdade de Ciências da Universidade do Porto

Se questionarmos a um químico sobre os ângulos que associa ao Carbono, possivelmente referirá,  $109.47^\circ$  ou  $120^\circ$ , os ângulos entre ligações carbono-carbono (C-C), na estrutura do diamante e da grafite, respetivamente.

A grafite é um empilhamento de camadas atômicas---grafeno---em que as ligações C-C formam ângulos de  $120^\circ$ ). As camadas partilham a mesma orientação, mas camadas sucessivas estão deslocadas de uma distância C-C. A bi-camada de grafeno é grafite com duas camadas. A ligação entre elas não é suficientemente forte para fixar a sua orientação relativa, e a bi-camada forma-se com um ângulo entre as orientações da cada camada (*twist*).

Os ângulos mágicos, são uma sequência de pequenos ângulos de twist, da ordem de  $1^\circ$  ou menos, que, surpreendentemente, dão à bi-camada propriedades físicas fascinantes, que nada têm a ver com a bi-camada sem twist (mesma orientação). Esta palestra versará sobre este sistema que tanto fascina os físicos de matéria condensada.



## REFERENCES

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- [2] M. Mrongovius, "Public engagement with hologram," in *11th International Symposium on Display Holography*, Aveiro, 2018.
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# **Sustentabilidade em cenários de alterações climáticas**

## **A contribuição da Física**

Filipe Duarte Santos (Univ. Lisboa)

A sustentabilidade envolve três dimensões essenciais que interatuam, designadamente as sociais, económicas e ambientais, incluindo nesta última a problemática da sobre-exploração dos recursos naturais e das alterações climáticas.

A interferência do Homo sapiens na biosfera está a afetar a sua integridade e a colocar em perigo os serviços dos ecossistemas que esta espécie biológica explora e dos quais depende. O conhecimento científico sobre o sistema Terra, e em particular sobre a biosfera, nunca foi tão abrangente e detalhado e, simultaneamente, a interferência humana no sistema Terra, e em especial sobre a biosfera, nunca foi tão intensa e transformadora, desde a escala local à global. O atual paradigma de desenvolvimento é baseado no uso intensivo de energia. Desde o princípio do século XVIII a energia foi assegurada maioritariamente pelos combustíveis fósseis o que tem o efeito colateral de provocar alterações climáticas. Como descarbonizar a economia mundial e simultaneamente assegurar fontes de energia abundantes e acessíveis?

Será apresentada uma breve história do conceito de sustentabilidade, dos desafios atuais e das soluções e caminhos para a atingir. Será dada especial relevância à importância da física e da investigação em física na caminhada para a sustentabilidade.



## **Buracos Negros: de uma Equação ao Nobel**

Carlos Herdeiro (Univ. Aveiro)

Nesta palestra iremos discutir alguns dos desenvolvimentos que marcaram um século de história dos buracos negros. Desde a sua génese nos primórdios da Relatividade Geral, como soluções das equações de campo de Einstein, mas consideradas irrealistas e mal compreendidas durante meio século; até ao seu entendimento teórico moderno, discutindo a sua evidência observacional acumulada ao longo do último meio século. Estes desenvolvimentos culminaram no Prémio Nobel da Física de 2020, que premeia desenvolvimentos cruciais relativos ao estudo teórico de buracos negros (metade do prémio atribuído a Roger Penrose) e da sua evidência observacional (metade do prémio atribuído a Reinhard Genzel e Andrea Ghez).

## **O Prémio Nobel de G. Parisi: Matéria Condensada, Desordem e Sistemas Complexos**

**Margarida Gama (Univ. Lisboa)**

O Prémio Nobel de G. Parisi: Matéria Condensada, Desordem e Sistemas Complexos.

A Física baseia-se em observações e propõe teorias para descrever fenómenos em todas as escalas. A “nossa” escala é o desafio da Física da Matéria Condensada, onde o balanço entre a ordem e a desordem determina a estrutura e as propriedades da matéria. É como se as peças de um jogo de LEGO pudessem escolher as formas (correlações) para construir estruturas com propriedades pré-definidas ou nunca imaginadas. Um desafio intelectual com aplicações ilimitadas!

O prémio Nobel de 2021 atribuído, em parte, a G. Parisi da Universidade da Sapienza de Roma, reconhece o seu trabalho na descrição do efeito da desordem em fases com uma ordem complexa, os vidros, em particular os vidros de spin (onde os graus de liberdade são magnéticos). Os vidros são exemplos de um tipo de matéria condensada caracterizada por desordem, mas que apesar disso pode apresentar ou apresenta uma ordem complexa. Foi exatamente a descoberta e a caracterização deste tipo de ordem que permitiu a Parisi resolver um modelo de vidros de spin e mudar para sempre a nossa compreensão dos sistemas complexos.

A descoberta de Parisi vai muito para além da caracterização de um novo tipo de ordem e tem inesperadamente (ou não) inúmeras aplicações, que vão desde a biologia às ciências da computação.



# **Implementación de proyectos STEAM. Descripción y análisis de su implementación en el aula de Secundaria**

**Miguel Ángel Queiruga Dios**

<sup>1</sup>Universidad de Burgos,09001 Burgos

Los currículos educativos se están orientando hacia un enfoque integrativo de las disciplinas [1,2]. Así, de un tiempo a esta parte, se habla de los enfoques educativos STEM (Science, Technology, Engineering and Mathematics) o STEAM, que busca la integración de las disciplinas STEM y el arte, el lenguaje, los estudios sociales y las humanidades [3].

Esta integración de las disciplinas permite abordar, además, la comprensión y resolución de problemas actuales, desde una mayor interdisciplinariedad [4]. Con esto, se contribuye a desarrollar la alfabetización científica del alumnado preparándolo para la ciudadanía global, a la par que enriqueciendo las experiencias de aprendizaje mejorando los aspectos afectivos del proceso de enseñanza-aprendizaje, disminuyendo el abandono escolar.

En esta comunicación se definirá qué es la educación STEAM o el enfoque educativo STEAM y algunas de las metodologías para su implementación en el aula. Además, se analizarán ejemplos reales de proyectos STEAM realizados por alumnado de Enseñanza Secundaria utilizando la metodología de Aprendizaje Basado en Proyectos/Problemas. También se apuntarán algunas dificultades que pueden surgir durante el proceso, como en la formación de equipos, el reparto de tareas o la evaluación de los productos; y se hablará de la importancia de crear conexiones o sinergias con el entorno.

Educational curricula are moving towards an integrative approach to disciplines [1,2]. Thus, for some time now, there has been talk of STEM (Science, Technology, Engineering and Mathematics) or STEAM educational approaches, which seek the integration of STEM disciplines and art, language, social studies and the humanities [3].

This integration of the disciplines also allows addressing the understanding and resolution of current problems, from a greater interdisciplinarity [4]. With this, it contributes to developing the scientific literacy of students, preparing them for global citizenship, while enriching

learning experiences by improving the affective aspects of the teaching-learning process, reducing school dropout.

This communication will define what STEAM education or the STEAM educational approach is and some of the methodologies for its implementation in the classroom. In addition, real examples of STEAM projects carried out by Secondary School students using the Project/Problem Based Learning methodology will be analyzed. Some difficulties that may arise during the process will also be pointed out, such as in the formation of teams, the division of tasks or the evaluation of products; and the importance of creating connections or synergies with the environment will be discussed.

## Referencias

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## Comunicação Orais

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## Ensino da Física

# DISTINGUISHED SCIENTISTS: FROM CREATIVITY TO KNOWLEDGE

**Ariza Montes, M. M.<sup>1</sup>, Henares Paredes, J. D.<sup>2</sup>**

<sup>1,2</sup> IES "Pedro Espinosa. Carrera de Madre Carmen, 12. 29200-Antequera (Málaga). Spain  
[matiariza@iespedroespinosa.es](mailto:matiariza@iespedroespinosa.es)

**Keywords:** scientists, scientific instruments, busts

Bringing scientists closer to the teaching of physics is essential to understand the reality in which they lived and their capacity to innovation with the available means to them. This research aims to promote the heritage from the school IES "Pedro Espinosa", examining scientific knowledge through its characters and promoting the life, work and figure of scientists, whose centuries-old instruments house this historical institute, to reinforce the teaching and dissemination of physics.

## Methodology

Different scientists have selected, who have developed a century-old scientific instrument exhibited in this school. Next, two types of actions have carried: scientific and artistic. On one hand, the life and work of these authors have investigated to learn about the trajectory that led them to the discovery of a law or the invention of a scientific instrument, making a scientific-historical analysis. On the other hand, the performance has focused more on his psychological profile to portray his appearance in the form of a bust, carried out by the students from Arts high school, in which it has been necessary to explore the images of the scientist, the clothing of the time, the Roman busts. In this way, each of the

scientists has sculpted on a frame, using terracotta, which has then hollowed out, fired at 900°C and finished with sandpaper and bronze patina paint. Finally, a trunk pedestal has created, so that they exposes in the school IES "Pedro Espinosa" next to the scientific instruments that they designed.



**Figure 1.** Benjamin Franklin: Sculpture and scientific instrument "Franklin heart rate monitor".

## Results and Discussion

The creation of the materials of each scientist differs depending on their bibliographic information. On the other hand, the difficulty of reflecting his image on the bust has been more complex in some models than in others, requiring some more tedious techniques to certain nuances of the expression of each figure. At the end, all the studies have reached its final product, since students have learned not only the professional facet of scientists but they have completed it through the busts made. These sculptures will be part of the permanent exhibition of scientific-historical instruments of our high school in Antequera and will published at the Virtual Museum of Heritage from the IES "Pedro Espinosa".

## References

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# PROTEÇÃO DOS OLHOS CONTRA A RADIAÇÃO ULTRAVIOLETA

**Luís Afonso<sup>1</sup>, Luis Peralta<sup>2</sup>**

<sup>1</sup>Laboratório de Instrumentação e Física Experimental de Partículas, Lisboa, Portugal; Agrupamento de Escolas de Benfica, Lisboa, Portugal.

lafonso@lip.pt

<sup>2</sup> Laboratório de Instrumentação e Física Experimental de Partículas, Lisboa, Portugal; Faculdade de Ciências, Universidade de Lisboa, Portugal.

luis@lip.pt

No contexto do desafio ‘Radiação Solar’ que abrange aprendizagens essenciais de cinco disciplinas (biologia, física, geografia, matemática e química) propõe-se a atividade experimental ‘Proteção dos olhos contra a radiação ultravioleta’. O uso de óculos de sol é importante em dias de grande luminosidade. Protegem os olhos da radiação visível e da radiação ultravioleta (UV). A radiação UV pode danificar a retina, por isso é importante bloquear a sua passagem. Os olhos possuem mecanismos de proteção, como fechar as pálpebras ou diminuir o diâmetro da pupila. Esses mecanismos são ativados na presença de luz visível intensa, portanto, filtrar apenas esse componente pode deixar os olhos desprotegidos da radiação UV. Neste trabalho reconstruímos e aprimoramos um dispositivo construído por um dos autores [1]. O dispositivo permite avaliar a redução da intensidade da luz visível e UV próxima introduzida pelas lentes coloridas. O componente fundamental desta montagem é um conversor de luz-tensão integrado com uma janela de sensibilidade que abrange desde o UV próximo ao infravermelho. Como fontes de luz, são usados LEDs de diferentes comprimentos de onda. Foram utilizadas lentes de óculos de marca compradas em óticas e óculos comprados em lojas de desporto. Aplicamos a atividade experimental a alunos do ensino secundário numa aula de física do 12º ano. Os testes não revelaram diferenças significativas entre os dois tipos de óculos ou entre as várias cores de lentes. Em geral, a experiência realizada mostrou que a proteção oferecida pelas lentes coloridas testadas é adequada para a região crítica de UV.

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# HOLOGRAPHIC OPTICAL INSTRUMENTS PRODUCTION AND HOLOGRAPHIC INTERFEROMETRY AS CONTENTS FOR LABORATORY PRACTICES FOR UNDERGRADUATE STUDENTS IN PHYSICS AND PHYSICS TEACHING

José Caiongo Chibaca<sup>1,2</sup>, Helder Crespo<sup>1</sup>

<sup>1</sup>IFIMUP-IN and Department of Physics and Astronomy, Faculty of Sciences, University of Porto,  
Rua do Campo Alegre 687,4169-007 Porto, Portugal

<sup>2</sup>departamento de Exact Sciences, Higher Institute of Education Sciences of Uíge, Rua do Café, Uíge, Angola  
[josechibaca@hotmail.com](mailto:josechibaca@hotmail.com); [up201502143@edu.fc.up.pt](mailto:up201502143@edu.fc.up.pt); [hccrespo@fc.up.pt](mailto:hccrespo@fc.up.pt)

## ABSTRACT

Since the invention of Holography by Dennis Gabor in 1947 [1] and with the invention of the laser by Maiman in 1960, several new holographic techniques and applications have been devised and others are still being developed today. These range from scientific research to technological applications, such as medical imaging techniques, and also in the field of education as well as in art and/or public engagement [2], where, a hologram is also seen as a way of communicating science and technology. The objective and the main purpose of this paper, is to explore the phenomena of interference and diffraction of laser light by producing holographic optical instruments and to apply interferometry principle to study holographic interferometry that can be incorporate to the laboratory practices contents for undergraduate students in Physics and Physics teaching. Three-dimensional (3D) display technologies are one of the most promising for the introduction of undergraduate students to basic optics courses [3] and as an art medium, where computer-generated hologram (CGH) technologies are also used. Various uses of holography have been suggested by different authors for application in the field of education, from physics outreach and as a teaching tool for holography itself [5, 6], in optical image processing classes [7], in optics courses in general [8] and for math contents [9], providing a wide range of possibilities for solidifying the knowledge of middle and high schools students [10] while introducing the basic concepts of optics and photonics. Optical Holography is the most used technique for the teaching of physics and/or public engagement because it helps understand the physics of interference of coherent light and is a very motivating tool for the teaching of applied optics and can be used just as effectively in outdoor popular science events as in higher level physics teaching [11]. Our experimental results obtained with a versatile setup based on a single-frequency diode-pumped solid-state laser [12] are presented in this paper. The experimental work was performed using advanced optical and optomechanical components within a laboratory setting. For that, two reflection holograms (holographic mirror and double exposure holographic interferometry) and one transmission hologram (holographic magnifying glass) were produced using multi-beam configuration. With this work, we believe that is possible to use it for the teaching of some physics contents if included in laboratory experiment classes.

**Keywords:** Holographic optical instruments; holographic interferometry; laboratory practices; Optics; Photonics.

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# PROGRAMA DE SIMULAÇÃO DE QUEDA EM FLUIDOS

**Rui Jorge Agostinho<sup>1</sup>, Ana Tavares Sousa<sup>2</sup>**

<sup>1</sup> Departamento de Física da Faculdade de Ciências da Universidade de Lisboa

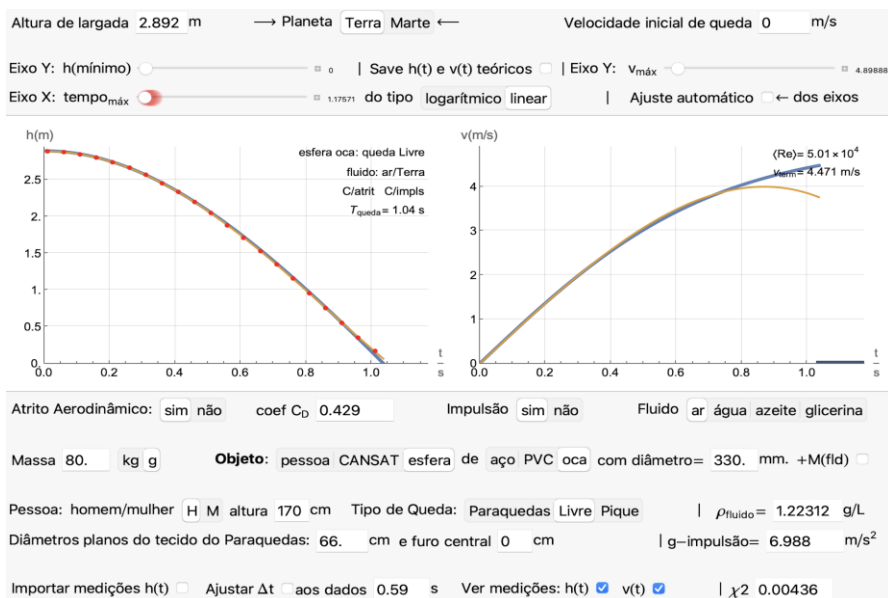
E-mail de contacto: [rjagostinho@fc.ul.pt](mailto:rjagostinho@fc.ul.pt)

<sup>2</sup> Escola Secundária do Restelo do Agrupamento de Escolas do Restelo

E-mail de contacto: [anatsousa@hotmail.com](mailto:anatsousa@hotmail.com)

As AE de Física e Química A referem o estudo de “*movimentos retilíneos como queda livre e queda com efeito de resistência do ar não desprezável, aplicando abordagens analíticas e gráficas*”. Para auxiliar este estudo em sala de aula, desenvolveu-se um programa em *Mathematica* (que corre no *Player*) que demonstra gráfica e interactivamente a solução das equações do movimento,  $h(t)$  e  $v(t)$ , para diversas condições de: aceleração gravítica, velocidade inicial, atrito aerodinâmico, fluido, impulsão, altura de queda e tipo de objeto em queda. O programa permite importar dados obtidos com um sensor de posição para sobrepor ao modelo teórico, ou mostrar tabelas de dados já nele incorporadas.

Esta ferramenta tem sido utilizada com sucesso quer em sala de aula, quer em programas extracurriculares como o CANSAT.



**Figura 1.** Interface do programa com a solução analítica (azul) para a queda duma bola de praia, associada às medições experimentais (pontos) e funções de ajuste (laranja).

# SPINS PRIMEIRO, PARA NÃO FICAR PARA TRÁS

Vítor S. Amaral,<sup>1</sup>

<sup>1</sup>Departamento de Física e CICECO, Universidade de Aveiro, Campus de Santiago, 3810-193 Aveiro  
email: vamaral@ua.pt

O ensino de Mecânica Quântica é considerado dos mais complexos no trajeto dum estudante de Física, sendo reconhecidas as principais dificuldades de compreensão conceptual [1,2], tolhida muitas vezes por complexidade matemática do tratamento. Nos cursos introdutórios, numa abordagem tradicional, os aspetos quânticos fundamentais e a sua imediata ligação a experiências basilares e aplicações tecnologicamente relevantes atualmente é muitas vezes relegada para o final, ou para estudos mais avançados. Mas há perspetivas de modernização.

A abordagem “spins-first”, de que Richard Feynman e Julian Schwinger foram pioneiros, na década de 60 do século passado, leva rapidamente o estudante a deparar com as características quânticas “estranhas” dos sistemas físicos, sem explicação clássica: sobreposição, entrelaçamento. Trabalhando inicialmente em espaços de dimensão finita e pouco mais que a álgebra vetorial e matricial elementar, esta abordagem imerge o estudante num vasto domínio de fenómenos e sua natureza aleatória, fornecendo intuição e bases sólidas de compreensão, transposta depois para em espaços de dimensão infinita com variáveis contínuas.

Por outro lado, uma abordagem que não segue uma linha histórica nem uma forma axiomática imperativa, e onde os conceitos quânticos e os requerimentos de representação (matricial e de Dirac) vão sendo incorporados progressivamente, em contextos fenomenológicos específicos, necessita duma sustentação metodológica adequada. Esta é já possível com simulações, demonstrações e experiências interativas disponibilizadas na Internet [3] que reforçam os aspetos interpretativos, sem paralelo e em conflito com a física clássica. Estas ferramentas têm a vantagem de poder ser aplicadas pelos estudantes, ao seu ritmo de trabalho, sendo a sua utilização orientada por guiões de trabalho tutorial.

Começando com sistemas de spin  $\frac{1}{2}$ , fótons únicos polarizados, e seguindo depois para sistemas de espaços compostos (mais do que uma partícula ou múltiplas variáveis) com correlações, esta abordagem fornece também as bases para estudantes em áreas afins da física, nas modernas aplicações tecnológicas, de informação e computação quânticas. Em vários países europeus, a modernização da educação quântica a nível secundário e de graduação inicial tem vindo ser reforçada, de formas ainda muito diversas e diferentes estádios de incorporação conceptual [4]. Motivar os jovens para a compreensão dos fenómenos, a manipulação de estados quânticos simples, e os fundamentos das tecnologias quânticas, é o objetivo da reformulação de cursos do 3º ano (Mecânica Quântica) e mais recentemente do 1º ano (Física Moderna). Será apresentada uma resenha das situações tratadas, seu encadeamento e progressão, bem como das atividades de interação, nos tutoriais e questionários de trabalho, promovendo e valorizando a autonomia dos estudantes.

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# CAPACIDADES TÉRMICAS: ASPETOS TEÓRICOS E DIDÁTICOS

**Joaquim Anacleto**

Departamento de Física, ECT, UTAD, Vila Real  
IFIMUP, Departamento de Física e Astronomia, FCUP, Porto  
email: anacleto@utad.pt

As capacidades térmicas a volume constante ( $C_V$ ) e a pressão constante ( $C_P$ ) são tópicos importantes, e estão incluídos em praticamente todos os currícula de Termodinâmica. Contudo, estes conceitos encerram algumas subtilidades que merecem ser analisadas, do ponto de vista científico e didático. Por exemplo, os índices  $V$  e  $P$  originam provavelmente confusões nos alunos, levando-os a questionar se  $C_V$  e  $C_P$  são propriedades do sistema ou do processo [1, 2]. Para além de prestarmos atenção às dificuldades evidenciadas em estudos focados nos alunos [3], implementando estratégias de ensino adequadas, é também necessário olhar para os aspetos conceptuais da teoria antes do ensino. Nesta comunicação, é evidenciado que  $C_V$  e  $C_P$  são propriedades do sistema, muito embora estas grandezas sejam usualmente introduzidas usando o calor, o qual é uma função do processo. É também mostrado que o trabalho dissipativo tem de ser incluído, juntamente com o calor, para se obterem definições corretas de propriedades do sistema, ou seja, o calor e o trabalho dissipativo produzem efeitos indistinguíveis no sistema. A pouca relevância dada na literatura ao trabalho dissipativo pode explicar algumas das dificuldades em termodinâmica [1, 2].

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**Joaquim Anacleto**

Departamento de Física, ECT, UTAD, Vila Real  
IFIMUP, Departamento de Física e Astronomia, FCUP, Porto  
email: anacleto@utad.pt

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# A CIÊNCIA POR DETRÁS DUM PÊNDBULO: INDO ALÉM DO PÊNDBULO FÍSICO

**Horácio Fernandes<sup>1</sup>**

<sup>1</sup> Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa  
[hf@ipfn.tecnico.ulisboa.pt](mailto:hf@ipfn.tecnico.ulisboa.pt)

## RESUMO

A “World Pendulum Alliance” é uma associação informal de instituições agrupadas em torno de uma oferta global de latitudes com pêndulos remotamente controlador e adequados para medições da gravidade local. Esta organização mundial foi construída sobre um software federado e de código aberto (Framework for Remote Experiments in Education - FREE), permitindo a autenticação do utilizador de modo a permitir a integração em Sistemas de Gestão de Aprendizagem (LMS ou CMS). Hoje em dia, inclui escolas secundárias (ensino médio), centros de ciência e universidades que disponibilizam através de servidores especializados várias experiências controladas remotamente. A maioria das escolas secundárias pertencem à rede das "Escolas Portuguesas no Estrangeiro" e as universidades estão localizadas na América Latina (Chile, Panamá, Brasil e Colômbia).

No entanto, esta constelação de pêndulos pode ser utilizada com outros propósitos, uma vez que o pêndulo é uma experiência única que permite alicerçar todo o ensino da mecânica.

Ao contrário das simulações, esta apresentação cobre aspetos “escondidos” que só podem ser observados pela experimentação, trazendo à tona características únicas resultantes de uma análise mais detalhada dos dados experimentais. Efetivamente, a precisão obtida por esta experiência é elevadíssima ( $3 \times 10^{-5}$ ) devido a uma seleção criteriosa de uma fotogate acionada diretamente por um laser e ainda devido ao elevado comprimento do cabo (~3m) e a massa do pêndulo (2kg). Além disso, uma leitura diferencial pode mesmo eliminar incertezas sistemáticas permitindo precisões quase uma ordem de grandeza acima. Aproveitando essa precisão, alguns efeitos mecânicos normalmente subestimados e/ou desprezados podem ser medidos e utilizados para ir mais além do simples pêndulo físico. Por exemplo pode-se explorar a deteção das marés gravíticas, a conservação da energia mecânica, o movimento angular e até mesmo o efeito de pêndulo de torção no cabo, medindo o seu módulo de elasticidade.

# ADIÇÃO DE ELEMENTOS MULTIMÉDIA EM APPLETS DE FÍSICA PARA ALUNOS COM DISLEXIA

Léo Rodrigues Macena dos Santos<sup>1</sup>, Paulo Simeão Carvalho<sup>2</sup>

<sup>1</sup> Faculdade de Ciências da Universidade do Porto, Rua do Campo Alegre, s/n, 4169-007 Porto  
[leo.r.m.santos@gmail.com](mailto:leo.r.m.santos@gmail.com)

<sup>2</sup> Departamento de Física e Astronomia, Unidade de Ensino das Ciências, IFIMUP, Faculdade de Ciências da Universidade do Porto, Rua do Campo Alegre, s/n, 4169-007 Porto  
[psimeao@fc.up.pt](mailto:psimeao@fc.up.pt)

Com os avanços tecnológicos dos últimos anos, a sociedade ocidental contemporânea está cada vez mais integrada pelas tecnologias digitais de informação e comunicação (TDIC), integração que acontece também na educação. Assim, surgem muitos objetos de aprendizagem (OA) todos os anos e que são digitais, reutilizáveis e compartilháveis [1]. No ensino da Física, os *applets* são OAs cada vez mais utilizados como simulações de fenómenos físicos [2]. Alunos com alguma dificuldade de aprendizagem especial (DAE), como dislexia ou discalculia, podem não conseguir explorar adequadamente essas simulações por dificuldades interpretativas dos elementos visuais e textuais [3]. A solução passa pela adaptação de OAs para alunos com essas deficiências a partir da substituição sensorial, adicionando um recurso multimédia que utiliza outra via de sensação do usuário para transmitir uma informação. Neste trabalho apresentamos dois *applets* integrando recursos audiovisuais para a substituição visual-auditiva. As simulações foram criadas utilizando o modelo de cascata revista [4], adaptado pelo autor.

Ambos os OAs têm sons específicos associados às alterações dinâmicas do fenómeno. Além disso, existe uma assistente virtual que faz a leitura de textos da simulação e informa alterações realizadas pelo usuário. As aplicações foram testadas com alunos dos ensinos médio (Brasil) e secundário (Portugal), com e sem dislexia.

Os dados desta investigação foram recolhidos por inquérito relativamente às suas impressões sobre o OA e a presença de sons nas simulações. Percebeu-se que os recursos multimédia tiveram impacto positivo na perspetiva do utilizador, visto que para a maioria dos alunos, os sons ou foram indiferentes (alunos sem dislexia), ou úteis para a interpretação dos textos e animação.

## Agradecimentos

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# ASTRONOMY PROJECTS AT SCHOOL: INTERDISCIPLINARITY IN SCIENCE TEACHING

Álvaro Folhas <sup>1,2</sup>

<sup>1</sup>NUCLIO – Núcleo Interativo de Astronomia e Inovação em Educação, Largo dos Topázios, 48, 3ª Frente 2785-817 São Domingos de Rana

<sup>2</sup>CITEUC – Centro de Investigação da Terra e do Espaço da Universidade de Coimbra, Observatório Geofísico e Astronómico, Almas de Freire - Sta Clara, 3040-004 Coimbra

Email: alvaro.folhas@nuclio.org

Astronomy is a Science that awakens curiosity for the unknown, and amazement in discovery. These are fundamental elements to mobilize students for Science, promoting an interdisciplinary vision through the connections between the different areas of knowledge. A project focused on Astronomy always has Mathematics and Physics in mind, but it can also cover Chemistry, Biology, Geography, Geology, ICT and Arts, especially if we associate it with Astronautics and Space Exploration. It is therefore important to bring Astronomy to School, either through the curriculum, or through small projects (within the scope of curricular autonomy) to mobilize knowledge, reinforce learning and develop skills. “Student research projects (...) provide a valuable opportunity for high school students to experience many of the joys and frustrations that make up the intellectual challenge of Science. Astronomy is one branch of Science that lends itself to student projects.”[1].

Project-based learning encourages students to adopt a new way of curriculum design, focused on student engagement, innovation, and creative problem solving. In addition to the advantages widely indicated for hands-on and mind-on activities, astronomy allows the use of low-cost resources, namely the traditional school supplies (cardboard, adhesive tape, markers, rulers and protractors) to make instruments, being therefore accessible to the student, promoting an awakening to everything around us, from the shadows to the apparent movement of the celestial vault. But today, we can benefit from a myriad of international projects of high didactic interest unknown to many teachers, which need to be disseminated. Projects such as LaSciL (Large Scientific Infrastructures Enriching Online and Digital Learning), which aims to associate large scientific infrastructures with school education for the production of digital educational content based on real scientific data, or the CliC-PoLiT focused on sustainability urban and light pollution, require pedagogical innovation that allow learning related to the real world, but already properly structured didactically in order to avoid excessive consumption of time and scientific know-how that make the strategy unfeasible[2].

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# PROJETO VLAB-FIS: UMA PROPOSTA PRÁTICO-LABORATORIAL INCLUSIVA PARA O ENSINO SECUNDÁRIO

**Natália Alves Machado,<sup>1</sup> Paulo Simeão Carvalho<sup>2</sup>, Frederico Alan de Oliveira Cruz<sup>3</sup>**

<sup>1</sup> Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, s/n, 4169-007 Porto  
email: [up201700283@g.uporto.pt](mailto:up201700283@g.uporto.pt)

<sup>2</sup> Unidade de Ensino das Ciências, Departamento de Física e Astronomia, FCUP, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, s/n, 4169-007 Porto

<sup>3</sup> Universidade Federal Rural do Rio de Janeiro, BR-465, Km 7 Seropédica, Rio de Janeiro.

Em 2015, a Organização das Nações Unidas aprovou a agenda “Objetivos de Desenvolvimento Sustentável” que inclui, entre os seus dezasseis objetivos globais, o desafio de “Assegurar a educação inclusiva, equitativa e de qualidade [...]” [1]. Esse objetivo será somente alcançado se, independente do nível de escolarização, duas condições forem respeitadas: (1) os estudantes com algum tipo de necessidade educativa especial dispõem de ferramentas e recursos adequados; (2) as metodologias utilizadas pelos professores sejam adequadas à realidade onde todos os estudantes, dividam o mesmo espaço de aprendizagem. Um exemplo da necessidade de um novo olhar sobre o processo educativo está relacionado com a situação de estudantes com mobilidade reduzida, que necessitam realizar atividades laboratoriais, algo fundamental na área científica. Visto que poucos materiais são adaptados a presença de indivíduos com a condição já citada, estes adotam, por vontade própria ou por imposição, um comportamento puramente passivo com a atividade que será realizada. Para promover uma mudança no processo de ensino e aprendizagem, em condições nas quais o estudante esteja impedido de realizar atividade manipulativa numa experiência, é que surge o projeto VLAB-FIS [2]. A ideia central do projeto é a construção de sequências didáticas para a componente experimental de Física, tendo como base a disciplina de Físico-Química do ensino secundário português, envolvendo: processos de gravação, construção e utilização de vídeos introdutórios; exploração das simulações computacionais; análise de vídeos com utilização de um *software* que permitem aos estudantes recolherem dados experimentais como numa experiência real. Para mostrar as potencialidades do projeto, neste trabalho é apresentado o processo de desenvolvimento de uma sequência didática de um tema curricular, e a sua aplicação com um estudante do 11º ano com Distrofia Muscular de Duchenne [3].

## Agradecimentos

Os autores agradecem à Fundação para a Ciência e a Tecnologia (FCT), projetos UIDB/04968/2021 e UIDP/04968/2021, e à Comissão Europeia, project ERASMUS+ 2019 -1-RO01-KA201-063169 (Science Connect), por financiarem este trabalho.

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## Physics activities developed in the project FisAstEE

**José Gonçalves<sup>1</sup>, Paulo Simeão Carvalho<sup>2</sup>, Luciano Medeiros<sup>3</sup>**

<sup>1</sup>Unidade do Ensino das Ciências, IFIMUP, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal ; email: [joseaagoncalves@gmail.com](mailto:joseaagoncalves@gmail.com)

<sup>2</sup>Unidade do Ensino das Ciências, Departamento de Física e Astronomia, IFIMUP, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal

<sup>3</sup>UFF/INFES Universidade Federal Fluminense, Instituto do Noroeste Fluminense de Educação Superior Av. João Jasbick, s/nº, Bairro Aeroporto Santo Antônio de Pádua – RJ, Brasil

There is a greater retention of scientific information by the children when their parents talk about the contents addressed in the classroom, even when they do not have a specific scientific knowledge [1]. Several authors [2][3][4] point out and describe the importance of parents to improve their children's learning and develop skills, as well as the influence they have on increasing interest in sciences. This project aims to raise the awareness of parents about the importance of science in people's life and how they can help to develop proactive attitudes towards science in young children.

In this way, we developed a series of Physics and Astronomy low-cost activities. Those activities are presented and built with the parents in training sessions with the scientist (Fig. 1). Parents will then replicate those activities at home with their own children.



**Figure 1.** One of training sessions with parents. They built a phone and a nail bed.

### Acknowledgements

The authors thank the Fundação para a Ciência e a Tecnologia (FCT), projects UIDB/04968/2021 and UIDP/04968/2021, and the European Commission, project ERAS-MUS+ 2019 -1-RO01-KA201-063169 (Science Connect), for funding of this work.

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# ATIVIDADES EXPERIMENTAIS VIRTUAIS NO ENSINO EXPERIMENTAL DA FÍSICA

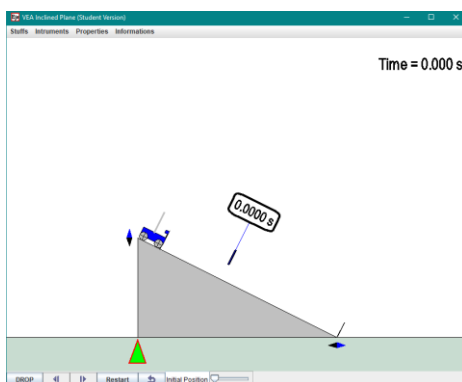
**M. Rodrigues,<sup>1,2</sup> P. Simeão Carvalho<sup>2,3</sup>**

<sup>1</sup> Agrupamento de Escolas António Sérgio, Av. Nuno Álvares, s/n, 4400 - 233 Vila Nova de Gaia, Portugal  
email: marcelojrodrigues@sapo.pt

<sup>2</sup> IFIMUP, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal

<sup>3</sup> Departamento de Física e Astronomia, Unidade de Ensino das Ciências, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal

As Simulações computacionais são ambientes digitais interativos que simulam fenómenos físicos reais e complexos [1]. Nestas simulações, por vezes o utilizador necessita de efetuar medições de grandezas físicas com instrumentos virtuais apropriados, para desta forma poder estudar e compreender o fenómeno. Neste trabalho apresentamos uma classe de simulações computacionais pedagógicas, as Atividade Experimentais Virtuais (AEV), que permitem desenvolver e promover, fora dos laboratórios, as competências dos estudantes relacionadas com os procedimentos experimentais e investigacionais, apoiando e complementando o ensino experimental nas escolas [2]. Tal como no mundo real, a recolha de dados está sujeita aos erros de medição aleatórios e sistemáticos, quer dos instrumentos de medida quer do próprio observador. Como exemplo, focar-nos-emos na AEV do Plano Inclinado (figura 1), uma atividade experimental que se enquadra nas aprendizagens essenciais do 10.º ano (variação da energia cinética com a distância percorrida) e no estudo da mecânica do 11.º ano.



**Figura 1.** Janela principal da AEV do Plano Inclinado (versão estudante).

Mostraremos que esta classe de simulações permite aos professores expandir a atividade experimental para fora do laboratório, enfatizando o método experimental, a recolha e análise de dados e o tratamento do erro experimental, complementando a atividade laboratorial real.

## Acknowledgements

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# COMO ORGANIZAR O ENSINO EXPERIMENTAL DE FÍSICA NA PÓS-PANDEMIA?

**J. Jorge Teixeira<sup>1</sup>, Lígia Teixeira<sup>1</sup>, Ana M. Dias<sup>2</sup>, Armando A. Soares<sup>3</sup>**

<sup>1</sup> Agrupamento de Escolas Dr. Júlio Martins, Av. 5 de outubro, 5400-017 Chaves, Portugal.

email: jjsteixeira@gmail.com

<sup>2</sup> Casio School Coordinator, Rua do Polo Sul, n.º 2 4.ªA, 1990-273 Lisboa, Portugal.

<sup>3</sup> Universidade de Trás-os-Montes e Alto Douro, Vila Real, Portugal.

O título desafia-nos para lógicas de ação antecipatória, relativamente a um futuro que, apesar de tudo, parece estar próximo. Estudos centrados nas consequências da pandemia identificam áreas prioritárias de atenção em competências estruturantes, como a resolução de problemas e o pensamento crítico e criativo [1], que o ensino experimental das ciências pode ajudar a desenvolver.

Neste contexto, este trabalho tem como principais objetivos sugerir e contextualizar algumas propostas relativas ao ensino experimental das ciências, em geral, e da Física em particular, que estão em implementação no Agrupamento de Escolas Dr. Júlio Martins, em Chaves, bem como apresentar o ponto de situação das mesmas.

As propostas tiveram por base o Plano 21|23 Escola+ e o relatório produzido pelo grupo de trabalho, de acordo com o Despacho n.º 3866/2021, de 16 de abril de 2021 [1]. As propostas parecem ter um impacto muito positivo na implementação contínua de abordagens e metodologias STEM pelos professores, na articulação vertical de conteúdos, na formação de professores na área do ensino experimental com calculadoras gráficas e sensores e no desenvolvimento de projetos científicos de âmbito escolar (figura 1).



**Figura 1.** Alunos a desenvolverem projetos e a apresentarem os resultados na sala STEM.

## Agradecimentos

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Eletrónica Flexível  
100 anos da experiência  
de Stern-Gerlach

## **Matéria Condensada**

# THEORY OF THE NONLINEAR OPTICAL CONDUCTIVITY

D. J. Passos,<sup>1</sup> J. M. V. P. Lopes,<sup>2</sup> J. M. B. Lopes dos Santos<sup>2</sup>

<sup>1</sup>Centro de Física Teórica e Computacional,

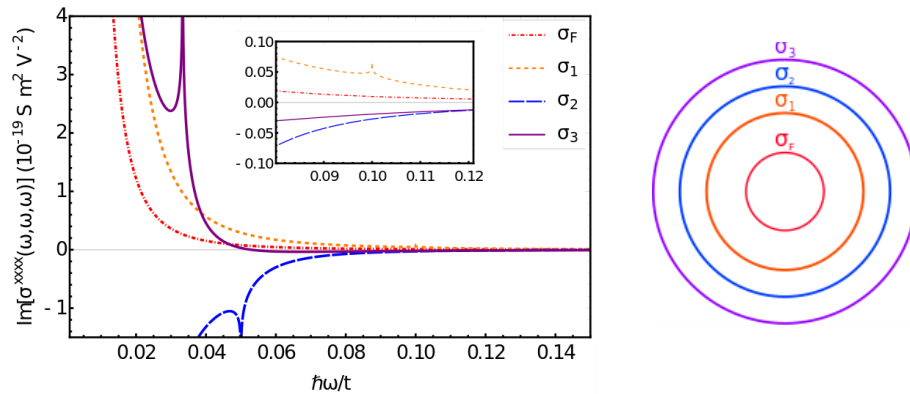
Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal

email: passos.djs@gmail.com

<sup>2</sup> Centro de Física das Universidades do Porto e do Minho,

Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, 4169-007 Porto, Portugal

The nonlinear conductivities, or susceptibilities, are response functions that encapsulate the nonlinear optical properties of materials observed under sufficiently intense laser light [1]. They are involved in describing everything in perturbative nonlinear optics, from second harmonic generation to the Kerr effect, self-focusing and even the more recently proposed jerk current [2]. Despite their central importance, the calculation of these quantities for crystals remains a challenge, partly due to the complexity of the perturbation theory involved. Here, this complexity is examined and recent advances are reviewed, with focus on electronic nonlinearities under the independent particle approximation. The resolution of a decades-long debate concerning gauge invariance (or lack thereof) is presented, as well as two methods of computation of nonlinear conductivities: a numerical algorithm based on a newly developed perturbation theory [3]; and a methodology for analytical derivations that follows from Aversa and Sipe's length gauge perturbation theory [4], but uses a resonance-based decomposition (Fig. 1) to reduce its complexity to a minimal set of "Fermi golden rule" type integrals and Hilbert transforms, with considerable gain in physical insight [5].



**Figure 1** On the left: resonance-based decomposition of the imaginary part of the third order conductivity (THG) of monolayer graphene. On the right: the different contributions probe different regions of the first Brillouin zone.

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# **Bose-Einstein Condensates in quasi-periodic lattices: bosonic Josephson junction and multi-mode dynamics**

**Henrique C. Prates<sup>1,\*</sup>, Dmitri A. Zezyulin<sup>2</sup>, Vladimir V. Konotop<sup>1</sup>**

<sup>1</sup>Centro de Física Teórica e Computacional and Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal.

<sup>2</sup>ITMO University, St. Petersburg 197101, Russia

\*email: hcprates@fc.ul.pt

Collective dynamics of two interacting spatially localized Bose-Einstein condensates (BECs) is one of the basic problems in the physics of condensed bosonic atoms. BECs confined in a double-well trap is a typical example, where one can find such fundamental phenomena, as coherent oscillations, spontaneous symmetry breaking, non-linear selftrapping, coupled solitons, etc. We show that an alternative, and in several aspects even more general, setting allowing the physical realisation of the mentioned phenomena is a BEC loaded in one-dimensional bichromatic optical lattices with constituent sublattices having incommensurate periods.

Using the rational approximations for the incommensurate periods, we show that below the mobility edge the localised states are distributed nearly homogeneously in the space. We obtain an alternative realisation of the bosonic Josephson junction, whose coherent oscillations display beatings or switching in the weakly nonlinear regime, as well as self-trapping. These phenomena can be observed for different pairs of modes, which are localised due to interference rather than due to the walls of the confining trap, providing a more general implementation of this junction. Furthermore, by considering several modes coupled by the nonlinearity, we investigate the four-mode dynamics, mimicking coherent oscillations and self-trapping in four-well potentials. The results obtained using few-mode approximations are compared with the direct numerical simulations of the one-dimensional Gross-Pitaevskii equation.

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# DIELECTRIC AND MAGNETIC PROPERTIES OF $\text{Ca}_3\text{Mn}_2\text{O}_7$ THIN FILMS

**Bruna M. Silva<sup>1</sup>, João Oliveira<sup>1</sup>, Tiago Rebelo<sup>1,3</sup>, Pedro Rocha-Rodrigues<sup>2</sup>,  
Neenu Lekshmi<sup>2</sup>, C. Amorim<sup>4</sup>, J. Amaral<sup>4</sup>, V. Amaral<sup>4</sup>, Armandina Lopes<sup>2</sup>,  
João Araújo<sup>2</sup>, Leonard Francis<sup>3</sup>, Bernardo Almeida<sup>1</sup>**

<sup>1</sup>CF-UM-UP, LAPMET, Univ. Minho, Campus Gualtar, 4710-057 Braga, Portugal, brunasilva@fisica.uminho.pt.

<sup>2</sup>INL, International Iberian Nanotechnology Laboratory, Av. Mestre José Veiga, 4715-330 Braga, Portugal.

<sup>3</sup>IFIMUP, LAPMET, Institute of Nanoscience and Nanotechnology and Photonics, Dep. Física e Astronomia, FCUP, Univ. Porto, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal.

<sup>4</sup>Physics Department and CICECO, Univ. Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal

Naturally Layered Perovskite structures with improper ferroelectricity [1, 2] such as the Rudlesden-Popper  $\text{Ca}_3\text{Mn}_2\text{O}_7$  allow exploring oxygen octahedra nonpolar rotations and cation site displacement to attain non-centrosymmetry. Furthermore, due to their high sensitivity to lattice-distortions, their preparation in thin film form over crystalline substrates allows the manipulation of acentricity and enables the tuning of lattice, electric and magnetic interactions. As such, thin films of calcium manganese oxide were prepared by pulsed laser deposition over  $\text{SrTiO}_3$  substrates, with different deposition conditions and post-deposition annealing steps. The A21am ferroelectric phase was observed in the films, along with the orthorhombic Acaa phase, with a preferential (111) growth direction. The magnetic properties were measured using a SQUID magnetometer, showing an antiferromagnetic (AFM) transition at 112 K (Fig. 1), characteristic of the  $\text{Ca}_3\text{Mn}_2\text{O}_7$  Rudlesden-Popper phase. The dielectric permittivity of the films shows the presence of dispersion described by the Havriliak-Negami model function with two relaxations. From temperature-dependent fits to the permittivity curves, a different behaviour of the parameters was observed when changing to the antiferromagnetic region. Additionally, the Kohlrausch-Williams-Watts stretched exponential parameter ( $\beta_{\text{KWW}}$ ) showed an abrupt decrease below  $\sim 112$  K, near the Néel temperature. This indicates the presence of magnetoelectric interactions and magnetically induced enhancement of dipolar-correlations in the AFM phase. The magnetic and dielectric properties of the films will be discussed and presented, highlighting the polar cooperative behavior and phase evolution and stabilization in the films.

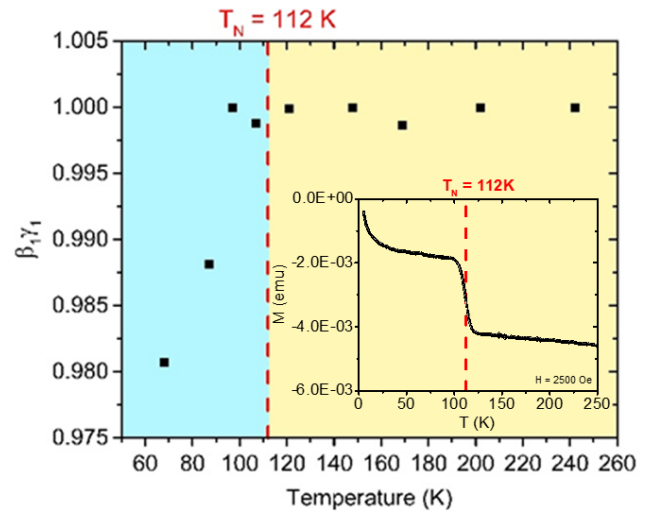


Figure 1. Temperature dependence of the stretched exponential parameter ( $\beta_{\text{KWW}}$ ) and temperature dependence of the magnetization (inset) marked with an abrupt decrease of observed below  $\sim 112$  K.

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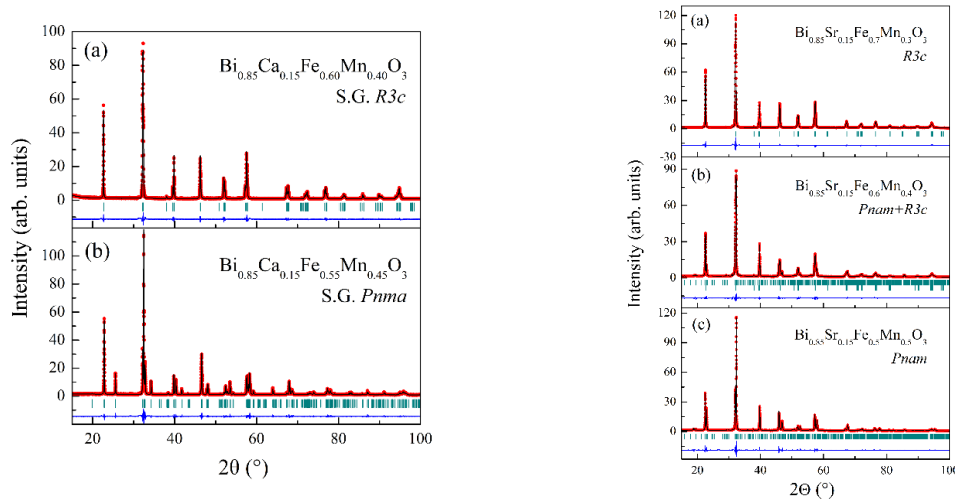


# Structural and Magnetic Transformations Induced by Mn Doping in Ca- and Sr- substituted BiFeO<sub>3</sub>

**M. Das<sup>1</sup>, J.A. Paixão<sup>1</sup>, V.A. Khomchenko<sup>1</sup>**

<sup>1</sup> CFisUC, Department of Physics, University of Coimbra, P-3004-516, Coimbra, Portugal  
email: [mithila.physics@gmail.com](mailto:mithila.physics@gmail.com)

Due to potential applications of magnetoelectric effect, the interest in bismuth ferrite (known as a multiferroic material with uniquely high transition temperatures ( $T_{AFM} \approx 640$  K,  $T_{FE} \approx 1100$  K) and very large spontaneous polarization ( $P_S \sim 100 \mu\text{C cm}^{-2}$ )) is growing steadily. This investigation focuses on the structural and magnetic correlations in Ca- and Sr- substituted bismuth ferromanganites. We use a doping scheme in which Fe<sup>3+</sup> ions are partially replaced by manganese in the mixed (Mn<sup>3+</sup>/Mn<sup>4+</sup>) oxidation state providing the ferromagnetic exchange coupling. The AE- substituted bismuth ferromanganites Bi<sub>0.85</sub>AE<sub>0.15</sub>Fe<sub>1-x</sub>Mn<sub>x</sub>O<sub>3</sub> (AE= Ca<sup>2+</sup> & Sr<sup>2+</sup> and  $0.1 \leq x \leq 0.5$ ) have been synthesized by a solid-state reaction method. It has been found that the ionic radius of an alkaline earth substituent,  $r$ , plays an important role in the structural evolution of the Bi<sub>0.85</sub>AE<sub>0.15</sub>Fe<sub>1-x</sub>Mn<sub>x</sub>O<sub>3</sub> perovskites. In the Ca- substituted series ( $r_{Ca^{2+}} < r_{Bi^{3+}}$ ), the increase in Mn concentration gives rise to the polar rhombohedral  $\rightarrow$  nonpolar orthorhombic ( $R3c \rightarrow Pnma$ ) structural phase transition (Fig. 1). In the Sr- substituted samples ( $r_{Sr^{2+}} > r_{Bi^{3+}}$ ), the increase of Mn content causes the polar to antipolar ( $R3c \rightarrow Pnam$ ) transformation (Fig. 1). Both Ca/Mn and Sr/Mn substitutions suppress the cycloidal magnetic modulation characteristic of the pure BiFeO<sub>3</sub> and induce the appearance of spontaneous magnetization [1, 2].



**Fig. 1.** Rietveld refinement of the XRD data collected for the Ca- and Sr- substituted BiFeO<sub>3</sub> at room temperature.

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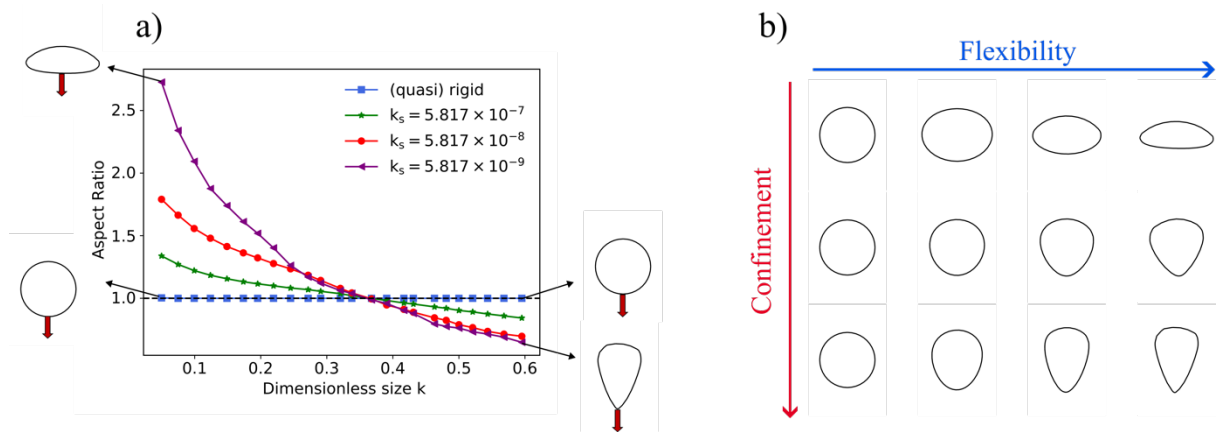
# Shape transition of sedimenting confined capsules

**Danilo P. F. Silva<sup>1,2</sup>, Rodrigo C. V. Coelho<sup>1,2</sup>, Margarida M. Telo da Gama<sup>1,2</sup> and Nuno A. M. Araújo<sup>1,2</sup>**

<sup>1</sup> Centro de Física Teórica e Computacional, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal; email: dpsilva@fc.ul.pt

<sup>2</sup> Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal

The transport of fluid-filled capsules under confinement constitutes an important problem with various applications from oil to pharmaceutical industries. The shape and dynamics of the capsule results from an interplay between flexibility, hydrodynamics and confining walls [1, 2]. We study the shape of deformable capsules under sedimentation in a quiescent viscous fluid inside a confined channel. We use a hybrid lattice Boltzmann method with immersed boundary (LBM-IB) to couple hydrodynamics with capsule shape and motion. For the membrane dynamics, we use a coarse-grained approach in which we use potentials to model the membrane stretching/bending energies and area constraints. We find that the shape of the capsule depends on the width of the channel and flexibility, with a shape transition from oblate-like to bullet-like shape, when the width of the channel is about two-thirds of the capsule diameter (see Fig. 1). We analyze the hydrodynamic stresses and forces responsible for this shape transition.



**Figure 1. (a)** Aspect ratio of capsules with different stretching coefficient  $k_s$  as a function of the dimensionless size  $k$ , defined as the ratio between capsule diameter and the width of the channel. Red arrow indicates direction of motion. **(b)** Collection of shapes as a function of flexibility and confinement.

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# The role of structural distortions in triggering the metal to insulator transition in NdNiO<sub>3</sub>

**Mariana M. Gomes<sup>1</sup>, Abdrazzak A. Bassou<sup>2</sup>, Manjunath Balagopalan<sup>1</sup>, Rui Vilarinho<sup>1</sup>, Bruna Silva<sup>3</sup>, João Oliveira<sup>3</sup>, Bernardo Almeida<sup>3</sup>, Abílio Almeida<sup>1</sup>, Pedro Tavares<sup>2</sup>, and J. Agostinho Moreira<sup>1</sup>**

<sup>1</sup> IFIMUP, Departamento de Física e Astronomia da Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal

email: up201402744@fc.up.pt

<sup>2</sup> Centro de Química-Vila Real, ECVA, Chemistry Department, Universidade de Trás-os-Montes e Alto Douro, 5000-801 Vila Real, Portugal

<sup>3</sup> CF-UM-UP, Departamento de Física, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal

Rare-earth nickelates, RNiO<sub>3</sub>, are challenging compounds due to their intriguing physics, consequence of the strong correlation between electronic, charge, spin and lattice degrees of freedom [1]. Among these compounds, NdNiO<sub>3</sub> has raised some controversy regarding the nature of its metallic to insulator transition (MIT). NdNiO<sub>3</sub> exhibits a first-order MIT, adopting a metallic and paramagnetic Pnma symmetry above  $T_{MI} = 200$  K and, in the insulating phase, transits into the P2<sub>1</sub>/n symmetry, with the stabilization of a E'-type antiferromagnetic phase [2]. In RNiO<sub>3</sub>, a close relationship between structure and MIT has been proposed due to the strong dependence of the  $T_{MI}$  from the rare-earth cation size [3]. The symmetry lowering at MIT is supposedly accompanied by NiO<sub>6</sub> breathing distortion that once coupled to in-phase and anti-phase octahedra rotation distortions would trigger the MIT. However, contrarily to smaller rare-earth cations, in NdNiO<sub>3</sub>, the amplitude of these oxygen rotations is not enough to stabilize the charge ordering and open the bandgap of the eg-Ni orbitals, and the magnetic ordering helps to promote the occurrence of MIT [3]. Therefore, in NdNiO<sub>3</sub>,  $T_{Néel} = T_{MI}$  is expected. While some experimental studies evidence the concomitant nature between structure and MIT [4], others completely reject it, assigning the magnetic ordering to the triggering mechanism instead [5]. The question still remains concerning the mechanisms that actual trigger MIT in NdNiO<sub>3</sub>.

Towards searching for an answer to this demand, we have carried out an experimental study in NdNiO<sub>3</sub> ceramics and thin films of 260 nm and 110 nm deposited onto (001) oriented LaAlO<sub>3</sub> substrate. In this work, we report temperature-dependent Raman scattering and magnetization measurements to follow the structure and magnetic order evolution across the MIT, which was identified from resistivity measurements. The experimental results point out for a decoupling between the structural and electronic orders but evidence a coupling between electronic and magnetic orders in NdNiO<sub>3</sub>, independently on the used sample type.

## Acknowledgements

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# Density Functional Theory and Perturbed Angular Correlation Study of the $AMnGe_2O_6$ (A=Be, Mg, Ca, Sr) Clinopyroxene Series

Ricardo Moreira<sup>1</sup>, Estelina L. da Silva<sup>1</sup>, <sup>7</sup>Alessandro Stroppa, Lei Ding<sup>6</sup>, Claire V. Colin<sup>4,5</sup>, Céline Darie<sup>4,5</sup>, Céline Goujon<sup>5</sup>, Murielle Legendre<sup>5</sup>, J. G. Correia<sup>2,3</sup>, Armandina M.L. Lopes<sup>1</sup>, João P. Araújo<sup>1</sup>

<sup>1</sup>IFIMUP, <sup>2</sup>CERN EP, <sup>3</sup>C2TN, <sup>4</sup>Univ. Grenoble Alpes, <sup>5</sup>CNRS, <sup>6</sup>ISIS Pulsed Neutron Facility, <sup>7</sup>CNR-SPIN

*e-mail: [ricardopachecomoreira@gmail.com](mailto:ricardopachecomoreira@gmail.com)*

Multiferroic materials have been under the spotlight due to their fundamental scientific interest and for potential applications in technology. Among these interesting materials are the group of compounds belonging to the Pyroxene family with general chemical formula  $AM(Si,Ge)_2O_6$ . More specifically,  $SrMnGe_2O_6$  [1] and  $CaMnGe_2O_6$ [2] are isostructural, crystallizing with monoclinic  $C_2/c$  symmetry and are characterized by zigzag chains of  $MnO_6$  octahedra linked by edge-sharing, separated by corner-sharing  $GeO_4$  tetrahedra chains along the same axis. Due to this arrangement these systems present a rich diversity of low-dimensional magnetic properties.

Since these properties might arise from local structural features that are not well described by methods based on long-range average structural models, the use of local probe studies is essential. In this context, hyperfine methods, such as perturbed angular correlation (PAC) spectroscopy where the study of the electric field gradient (EFG) in the vicinity of a probe atom, allows for the reconstruction of the atomic and electronic environment of the probe in the material, helps to clarify the origin of the properties exhibited in these systems.

In this work a temperature dependent EFG study will be presented and discussed, guided by EFG simulation results using Quantum ESPRESSO [3], attempting to clarify the nature of the two distinct local environments that are experimentally observed. Additionally, the electronic properties of these systems, as determined by DFT, will also be presented, along with those of the hypothetical compounds  $BeMnGe_2O_6$  and  $MgMnGe_2O_6$  which have yet to be experimentally realised.

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# PERCOLATION BASED SIMULATION TO PREDICT CAKING KINETICS OF POLYDISPERSED AMORPHOUS POWDERS

Vasco C. Braz,<sup>1</sup> André F. V. Matias,<sup>1, 2</sup> Laurent Forny,<sup>3</sup> Delphine Pasche,<sup>4</sup> Vincent Meunier,<sup>4</sup> Jan Engmann,<sup>4</sup> Nuno A. M. Araújo<sup>1, 2</sup>

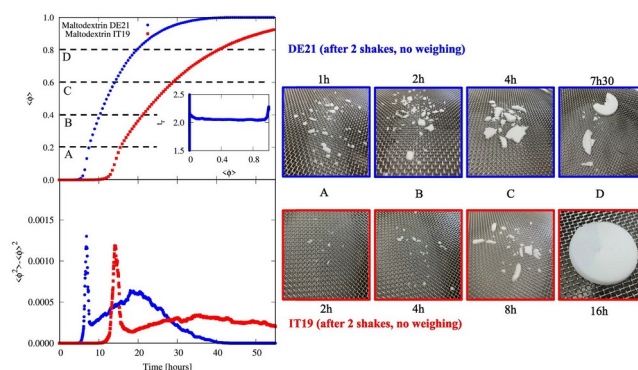
<sup>1</sup>Centro de Física Teórica e Computacional, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal; email: vc Braz@fc.ul.pt

<sup>2</sup>Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal

<sup>3</sup>Nestlé Product Technology Center Beverage, Route de Chavornay 3, 1350 Orbe, Switzerland

<sup>4</sup>Nestlé Research, Vers-chez-les-Blanc, PO Box 44, 1000, Lausanne 26, Switzerland

The shelf life of powder-based food products is usually limited by the dynamics of caking. Individual particles absorb water vapor, which triggers the formation of sinter bridges and the growth of lumps of particles, affecting the mechanical properties and perceived quality of the powder. Previous models of caking have focused on the dynamics at the particle level. To study the impact on global connectivity and mechanical properties, we mapped caking into a ranked percolation model where the formation of bridges is a non-trivial function of space and time. Since this threshold only depends on the geometry of the granular assembly, we can separate the contribution of the spatial heterogeneities and of the individual particle properties. This enables a rational approach for interpreting and mitigating caking propensity of commercial products consisting of particle species with different particle size distributions. We corroborate the numerical and analytical predictions with experiments.



**Figure 1.** Evolution of the order parameter  $\langle \phi \rangle$  (size of largest cluster) and the fluctuations  $\langle \phi^2 \rangle - \langle \phi \rangle^2$  for Glucidex DE21 (blue) and Glucidex IT19 (red). Right: Snapshots of the experimental realization of a moisture shock for Glucidex DE21 (blue) and Glucidex IT19 (red) for different times. The letters A, B, C, and D indicate similar states of the system for the different samples.

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## Física Nuclear

# ANALYSIS OF GAN CORE-SHELL P-N JUNCTION NANOWIRE RADIATION DETECTORS IRRADIATED WITH PROTONS

**D. Verheij<sup>1,4</sup>, L. C. Alves<sup>2,3</sup>, M. Peres<sup>1,3,4</sup>, S. Cardoso<sup>1</sup>, E. Alves<sup>3,4</sup>, C. Durand<sup>5</sup>, J. Eymery<sup>6</sup>, K. Lorenz<sup>1,3,4</sup>**

<sup>1</sup>Instituto de Engenharia de Sistemas e Computadores - Microsistemas e Nanotecnologia, Lisboa, Portugal, email: dverheij@inesc-mn.pt

<sup>2</sup>C2TN, Campus Tecnológico e Nuclear, Instituto Superior Técnico, Bobadela LRS, Portugal

<sup>3</sup>DECN, Campus Tecnológico e Nuclear, Instituto Superior Técnico, Bobadela LRS, Portugal

<sup>4</sup>IPFN, Campus Tecnológico e Nuclear, Instituto Superior Técnico, Bobadela LRS, Portugal

<sup>5</sup>CEA, IRIG, PHELIGS, NPSC, Université Grenoble Alpes, Grenoble, France

<sup>6</sup>CEA, IRIG, MEM, NRS, Université Grenoble Alpes, Grenoble, France

Gallium nitride (GaN) nano- and microwires have gained increasing interest due to their unique geometry and flexibility, and have already been successfully applied in optoelectronics. One important advantage is their superior crystalline quality in comparison to their thin-film counterparts. Beside this, GaN is also known for its high radiation hardness, owed to the large displacement energy of the atoms in its crystal lattice and efficient dynamic annealing properties.

In this work, single GaN core-shell p-n junction microwires have been processed into radiation detectors and it was already shown that these are capable of sensing UV light and ionizing radiation [2]. However, it is relevant to quantify precisely what the impact of the ionizing radiation on the electrical properties of the sensors is, namely compared to their silicon counterparts. Therefore, the detectors were irradiated using 2 MeV protons up to different fluences, more specifically in the range of  $5 \times 10^{13}$  protons/cm<sup>2</sup> to  $1 \times 10^{16}$  protons/cm<sup>2</sup>, while measuring the dark, photo- and ionocurrent *in-situ*. Furthermore, the photoconductivity before and after irradiation is compared.

The results show that for fluences up to  $1 \times 10^{14}$  protons/cm<sup>2</sup> there is no significant modification of any of the parameters. For fluences above  $5 \times 10^{14}$  protons/cm<sup>2</sup> the photo- and ionocurrent start to decrease and the reverse bias leakage current starts to increase, reducing the signal-to-dark current ratio significantly and indicating introduction of defects in the crystal lattice of the microwires. Nonetheless, only when the fluence exceeds  $1 \times 10^{16}$  proton/cm<sup>2</sup>, the detectors start to show serious deterioration, eventually leading to breakdown of the p-n junction properties. Additionally, EBIC measurements performed on irradiated samples show that a reduction of the space-charge region occurs as a consequence of the irradiation damage.

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# Cr-DOPED $\beta$ -Ga<sub>2</sub>O<sub>3</sub>: LUMINESCENCE ACTIVATION BY IRRADIATION-INDUCED DEFECTS

**D. M. Esteves<sup>1,2\*</sup>, M. Peres<sup>1,2,3</sup>, A. L. Rodrigues<sup>4</sup>, X. Biquard<sup>5</sup>, J. Zanoni<sup>6</sup>, J. Rodrigues<sup>6</sup>,  
N. Ben Sedrine<sup>6</sup>, B. M. S. Teixeira<sup>6</sup>, L. C. Alves<sup>3,4</sup>, M. I. Dias<sup>3,4</sup>, E. Alves<sup>2,3</sup>, Z. Jia<sup>7</sup>,  
W. Mu<sup>7</sup>, N. A. Sobolev<sup>6</sup>, M. R. Correia<sup>6</sup>, T. Monteiro<sup>6</sup>, K. Lorenz<sup>1,2,3</sup>**

<sup>1</sup> INESC MN, Rua Alves Redol, 9, 1000-029 Lisboa, Portugal

<sup>2</sup> IPFN, Instituto Superior Técnico, Av. Rovisco Pais, 1, 1049-001 Lisboa, Portugal

<sup>3</sup> DECN, Instituto Superior Técnico, University of Lisbon, EN 10, 2695-066 Bobadela LRS, Portugal

<sup>4</sup> C<sup>2</sup>TN, Instituto Superior Técnico, EN 10, 2695-066 Bobadela LRS, Portugal

<sup>5</sup> Université Grenoble Alpes, CEA, IRIG, MEM, NRS, 38000 Grenoble, France

<sup>6</sup> i3N, Departamento de Física, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal

<sup>7</sup> State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, People's Republic of China

\*Corresponding author — email: duarte.esteves@tecnico.ulisboa.pt

$\beta$ -Ga<sub>2</sub>O<sub>3</sub> is an emerging wide band gap semiconductor with promising applications, which include transparent conducting films for optoelectronic devices, solar-blind ultraviolet photodetectors and sensors. Due to its high transparency (wide band gap of  $\sim 4.9$  eV at room temperature — RT), it is a good host material for optically active centres in the spectral region spanning from the ultraviolet (UV) to the near-infrared (NIR). In particular, besides the characteristic UV/blue luminescence of undoped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, Cr doping provides efficient red/NIR light emission. At RT, the latter emission is dominated by two sharp lines (known as the R-lines) overlapped on a broad band; these can be assigned to the  ${}^2E \rightarrow {}^4A_2$  and  ${}^4T_2 \rightarrow {}^4A_2$  Cr<sup>3+</sup> intraionic transitions, respectively. In this work, we studied the modification of the optical properties of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> single-crystals doped with Cr or with Cr and Mg (Cr/Mg-doped) upon proton irradiation. The iono- and photoluminescence spectra of pristine Cr-doped samples were observed to be dominated by the UV/blue emission; however, during proton irradiation, this luminescence was progressively quenched, while the Cr<sup>3+</sup> emission was enhanced. In contrast, for Cr/Mg-doped samples, the Cr<sup>3+</sup> emission yield was already high in pristine samples, with no further increase occurring during irradiation. The two sets of samples also displayed distinct behaviours under thermoluminescence (TL) measurements monitored at the Cr<sup>3+</sup> emission wavelengths: while pristine Cr/Mg-doped samples showed strong TL signals, Cr-doped samples revealed no such signal prior to the proton irradiation. In fact, TL was activated in the latter samples after proton irradiation and quenched after thermal annealing at 650 °C. X-ray absorption near edge structure measurements suggest that the Cr charge state was not affected by the proton irradiation, invalidating the hypothesis that changes in the Cr charge state led to the enhancement of the Cr<sup>3+</sup> emission. Alternative mechanisms, including charge/energy transfer paths involving defect levels, will be discussed. Therefore, this study contributes to a better understanding of the defect levels that can sensitise the Cr<sup>3+</sup> luminescence in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, thus revealing the potential of Cr-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> for optical detectors of ionising radiation, both *in* and *ex situ*.

## Acknowledgements

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100 anos da experiência  
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## Óptica e Lasers

# Optical Tweezers development as a tool for biomedical diagnosis

**J. Freitas Oliveira<sup>1,2</sup>, Vicente Rocha<sup>1,2</sup>,  
Nuno A. Silva<sup>1,2</sup>, Pedro A. S. Jorge<sup>1,2</sup>**

<sup>1</sup>Departamento de Física da Faculdade de Ciências da Universidade do Porto

<sup>2</sup>Center for Applied Photonics (CAP), INESC-TEC

The use of single-beam gradient force trap, also known as optical tweezers, in biology and medicine, is widely known by the scientific community [1][2]. Ever since its inception in 1970, the optical tweezers setup has proven itself to be a reliable and versatile way of analyzing and classifying particles in a medium with relatively inexpensive equipment, eventually earning the creator, Arthur Ashkin, the Nobel Prize in Physics in 2018. With this technique, we attempt to identify and classify the state of nano Molecular Imprinted Polymers (nanoMIPs), distinguishing between bound and unbound status relative to a protein, such as an antibody [3]. This is achieved using a quadrant photodetector to capture the forward scattered light originated from the trap and scanning the position of the particle, which is then analyzed by machine learning algorithms (Principal Component Analysis and K-Nearest Neighbor) to determine the state. Preliminary results using PMMA beads ( $d=5\mu\text{m}$ ) bound to a protein (streptavidin) showed an accuracy of around 83%, making this method a potential suitable choice for biomedical detection and diagnosis tool.

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# OPTICAL PROPERTIES OF ONE-DIMENSIONAL PERIODIC STRUCTURES: FROM PHOTONIC CRYSTALS TO HYPERBOLIC METAMATERIALS

Bernardo Dias<sup>1</sup>, Luís C. C. Coelho<sup>1</sup>, and J. M. M. M. de Almeida<sup>1,2</sup>

<sup>1</sup> INESC TEC - Institute for Systems and Computer Engineering, Technology and Science, and FCUP, Univ. of Porto, R. do Campo Alegre, 4169-007 Porto, Portugal

<sup>2</sup> Dep. of Physics, Univ. of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal

Photonic crystals (PCs) consist of structures that create a periodic spatial modulation of the refractive index, leading to the formation of band gaps in the spectral window. These devices represent an optical analog of crystalline lattices in condensed matter physics since Bloch's theorem is applicable in both cases. These similarities have been thoroughly explored and led to the observation of Bloch Surface Waves [1], which consist of an analog of the Tamm states in a crystal. In the case of 1D PCs, these devices generally consist of a unit cell made of two dielectric materials with high and low refractive indices, with each unit cell of approximately the same length as the wavelength of the incident light. Photonic crystals have been employed in optical sensors, filters and high reflectance coatings [2].

Hyperbolic metamaterials (HM) consist of periodic anisotropic artificial materials displaying components of the effective dielectric tensor with opposite signals, meaning that their behavior can be seen as a metal or a dielectric depending on the orientation of the incident light. In the particular case of 1D HM, these structures consist of a periodic repetition of a dielectric-metal unit cell which is much smaller than the wavelength considered, allowing analysis with effective medium approximations. Nevertheless, an evaluation of their properties can also be done using the same formalism as in PCs [3], displaying much more accurate results and allowing a better understanding of the physics behind these structures.

In this work, the optical properties of one dimensional periodic layered media are presented, providing physical insight to their behavior. A comparison between PCs and hyperbolic metamaterials is made, establishing the differences and potentialities of both structures. Lastly, the application and comparison of both optical lattices as optical chemical sensors and biosensors are done, using the properties referred previously as a basis for the device design.

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# OPTICAL FIBER SENSOR FOR MEASURING WATER VAPOUR SORPTION HYSTERESIS OF CEMENT PASTE

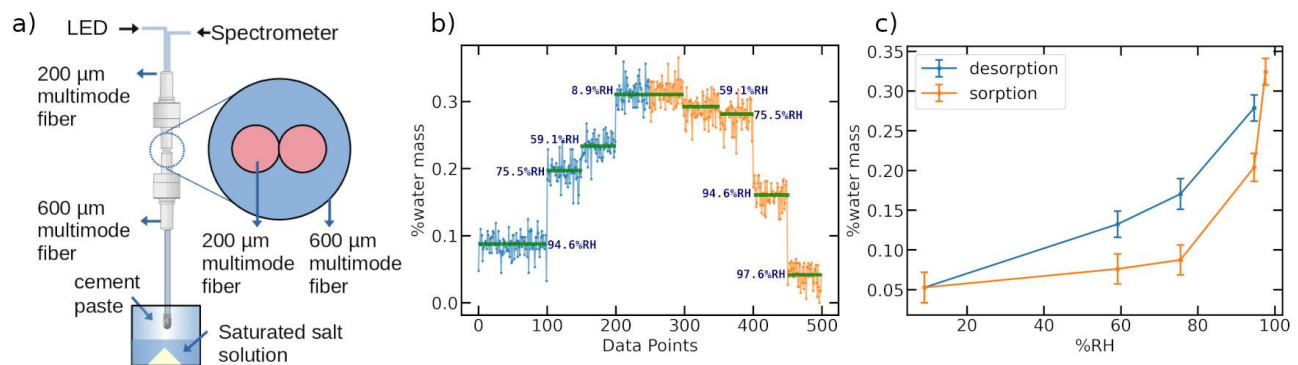
**P. M. da Silva<sup>1</sup>, Luís C. C. Coelho<sup>1</sup> e J. M. M. M. de Almeida<sup>1,2</sup>**

<sup>1</sup>INESC TEC-Institute for Systems and Computer Engineering, Technology and Science, and Faculty of Sciences, University of Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal

email: pedro.m.madeira@inesctec.pt

<sup>2</sup>Department of Physics, School of Sciences and Technology, University of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal

Monitoring water vapor sorption hysteresis (WVSH) is a powerful method of obtaining information from cement paste [1]. In it, water molecules are used as probes to estimate physical parameters and transport properties of cement paste. In this work we aimed to monitor WSVH through a multimode fiber embedded in the cement paste, Fig. 1a). Previously, the same monitoring scheme was used to achieve the capillary coefficient from the ingress and egress of water in the cement paste [2]. Cement paste's sorption or desorption of water occurs according to the relative humidity (RH) of the surrounding environment. The change in refractive index from the buildup of water at the fiber tip of the multimode fiber will decrease the amount of light being reflected at the fiber tip. Saturated salt solutions were used to achieve atmospheres with stable RH. The WSVH was successfully monitored at the fiber tip Fig. 1b-c), with estimates of pore distribution and cement paste's specific area being in accordance with the literature.



**Figure 1.** a) Setup used [2], b) light intensity converted to % water mass and its hysteretic behavior in c).

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# DEVELOPMENT OF A BIOGENIC AMINE OPTIC SENSOR USING ROSAMINE IN A CELLULOSE MEMBRANE

**Simão Seixas<sup>1\*</sup>, Luís C. C. Coelho<sup>1</sup>, Andreia Leite<sup>2</sup>, S. O. Ribeiro<sup>2</sup>, João Mendes<sup>1,3</sup> and J. M. M. M. de Almeida<sup>1,4</sup>**

<sup>1</sup>INESC TEC - Institute for Systems and Computer Engineering, Technology and Science, and Faculty of Sciences, University of Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal.

<sup>2</sup>LAQV-REQUIMTE, FCUP, University of Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal

<sup>3</sup>CIQUP – Chemistry Research Unit, Chemistry and Biochemistry Department, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal.

<sup>4</sup>Department of Physics, University of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal

\* Correspondence: simao.p.seixas@inesctec.pt

Biogenic Amines (BAs) are biomolecules produced by specific microorganisms and frequently found in food products. They result from metabolic reactions of microorganisms thus, their concentration is a good indicator of food spoilage. Besides the fact that they can lead to poisoning when consumed, the most used methods for their quantitative analysis have the disadvantages of requiring expensive equipment, specialized personnel and being time-consuming. This makes the development of new biosensors a great alternative since they are cheap and sensitive devices that allow for quick detection [1].

A biosensor for BAs detection may be feasible through a colorimetric membrane. A thin membrane of cellulose mixed with a rosamine pigment has been studied, which in contact with BAs, breaks the  $\pi$ -conjugation of the xanthene moiety, changing the macroscopic color of the membrane and its colorimetric characteristics [2].

In this work it was possible to access the colorimetric changes of the membrane in the presence of ethanol and ammonia. A transmission dip probe fiber bundle (from Avantes) and the membrane were placed in the optical path. While exposing the membrane to the active agents, a decrease in absorbance was detected over time when compared to the reference before the exposure, which confirms the predicted behavior of the membrane losing its color. The response time was short, and the process proved to be fully reversible after the removal of the active agent, recovering its original colorimetric properties. These results show that, with a higher selectivity, this biosensor has the potential to become a cheaper and more practical replacement for today's methods of BAs detection.

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# DEVELOPMENT OF AN OPTICAL MAGNETIC FIELD SENSOR BASED ON SURFACE PLASMON RESONANCE AND MAGNETOSTRICTION

João P. M. Carvalho<sup>1,2</sup>, Bernardo Dias<sup>1,2</sup>, Luís C. C. Coelho<sup>1,2</sup> and J. M. M. M. de Almeida<sup>1,3</sup>

<sup>1</sup> INESC TEC - Institute for Systems and Computer Engineering, Technology and Science, and FCUP, Univ. of Porto, R. do Campo Alegre, 4169-007 Porto, Portugal

<sup>2</sup> FCUP, University of Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal

<sup>3</sup> Dep. of Physics, Univ. of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal

The measurement of magnetic fields (MFs) is of extreme importance in research and industrial applications. Parasitic MFs can severely damage data storage devices, and many medical imaging techniques require control of MFs. Conventional electromagnetic (EM) sensors may present the obvious disadvantage of being influenced by MFs, therefore, optical-based sensors are an alternative, as they are immune to EM fields and are capable of operation under harsh environmental conditions [1].

Surface plasmon polaritons (SPP) are EM modes that form and propagate on the surface of a metal-dielectric interface. These EM modes are triggered by the surface plasmon resonance (SPR) of conduction electrons that occurs for EM excitation at given wavelengths. Changing the interface materials, their thicknesses or effective indexes will shift the SPR wavelength [2]. Magnetostriction is a property of magnetic materials in which a mechanical strain is induced by the presence of a MF. This strain causes volumetric expansions/contractions, tuning the sample's dimensions in a particular direction.

In this work, different configurations of multilayer thin films containing a magnetostrictive material are simulated, using the transfer matrix method [3], for the optimal sensitivity and visibility of the SPR wavelength shift for different thicknesses of the magnetostrictive material, that is expected to change with the applied MF. An optimal configuration was reached with a Ag/Fe/Si thin film. Preliminary studies about the effect of MFs on the SPR thin film structure fabricated by sputtering technique deposition will be presented.

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# DEVELOPMENT OF OPTICAL GAS SENSORS BASED ON POROUS MATERIALS

**Mariana A. F. de Melo e Sousa<sup>1,2</sup>, Bernardo Dias<sup>1,2</sup>, João P. Mendes<sup>1,3</sup>, José M. M. M. de Almeida<sup>1,4</sup>, Carla Queirós<sup>5</sup>, Andreia Leite<sup>5</sup>, Ana M. G. Silva<sup>5</sup>, Luís C. C. Coelho<sup>1</sup>**

<sup>1</sup> INESC TEC - Institute for Systems and Computer Engineering, Technology and Science, and Faculty of Sciences, University of Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal.

<sup>2</sup> Department of Physics and Astronomy, FCUP, Univ. of Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal

<sup>3</sup> CIQUP - Chemistry and Biochemistry Department, FCUP, University of Porto, 4169-007 Porto, Portugal.

<sup>4</sup> Department of Physics, University of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal

<sup>5</sup> LAQV-REQUIMTE, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal

\*Correspondence: marianademeloesusoua@gmail.com

Monitoring gases in a given environment is increasingly important not only to assess its toxicity levels, but also to control the presence of impurities, contaminants or leak detection in pipes or storage facilities. As most gases are odorless and are undetected by the human senses, the existence of sensor systems able to monitor its levels in the atmosphere play a crucial role in protecting human health and safety and preventing explosions and other catastrophic events [1].

Optical fiber sensors (OFS) allow the measurement of concentrations of gases combined with structures specially designed for this purpose, such as Metal-Organic Frameworks (MOFs) which exhibit high porosity, high degree of crystallinity and exceptional chemical activity. The porosity of the MOFs allows the capture of specific molecules, originating changes in optical properties, either through emission of fluorescence or displacement of the absorption band [2, 3].

In this work, a preliminary experimental investigation is presented on the detection of different gases using special optical fiber configurations, based either on plasmonic effects or in waveguide coupling between the fundamental mode and higher order cladding modes, and coated with the developed MOFs dissolved in PVA, Hidrogel and celulose.

## Acknowledgements

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# NANOSTRUCTURES TOWARDS NEAR INFRARED SENSING

Paulo S. S. dos Santos<sup>1,2</sup>, J. M. M. de Almeida<sup>1,3</sup>, I. Pastoriza-Santos<sup>4,5</sup> and  
Luís C. C. Coelho<sup>1</sup>

<sup>1</sup> INESC TEC - Institute for Systems and Computer Engineering, Technology and Science, and FCUP, Univ. of Porto, R. do Campo Alegre, 4169-007 Porto, Portugal

<sup>2</sup> FEUP, University of Porto, R. Dr. Roberto Frias, 4200-465 Porto, Portugal

<sup>3</sup> Dep. of Physics, Univ. of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal

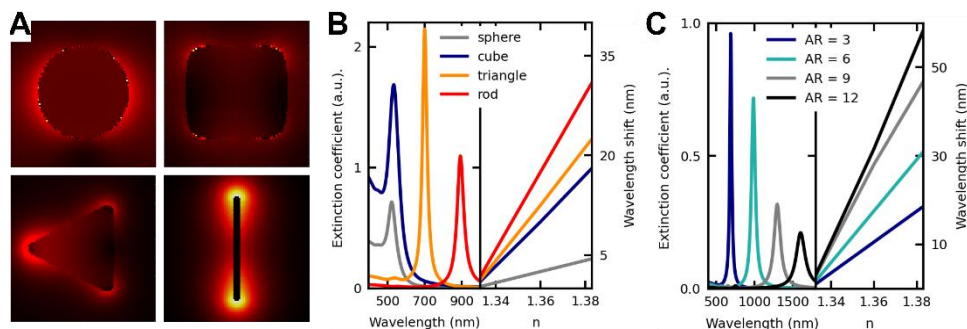
<sup>4</sup> CINBIO, Univ. de Vigo, Campus Univ. Lagoas, Marcosende, 36310 Vigo, Spain

<sup>5</sup> SERGAS-UVIGO, Galicia Sur Health Research Institute, 36312 Vigo, Spain

Nanoparticle (NP) assisted plasmonic bio and chemical sensing performance is highly dependent on their size, shape, and nanomaterial. The tailoring of those parameters allows the development of plasmonic sensors that can operate from ultra-violet (UV) to the near infra-red (NIR) regime [1]. The latter is of high importance in the implementation of plasmonic sensing with commonly available single-mode optical fibers at C-telecommunications band.

To achieve such goal is of primal importance to understand how the electromagnetic (EM) field enhancements and charge distribution profile on the NP is related to its spectral behavior, Fig. 1(a). These features allow to change their main plasmonic resonance towards higher wavelengths, along a greater refractive index (RI) sensitivity, Fig. 1(b). Sharper features also allows for greater EM enhancements. Such properties aid the design of plasmonic sensing at the NIR. As for nanorods, an aspect-ratio (AR) around 10 suffices to shift the plasmonic band towards 1500 nm, with increased RI sensitivity, Fig 1(c).

In this work, feasible routes to achieve plasmonic sensing towards NIR wavelengths were studied. Numerical work was conducted within the Boundary Element Method (BEM) approximation, to design such nanostructures, as well as experimental research via the colloidal synthesis of such nanostructures.



**Figure 1.** Plasmonic behavior comparison between Gold nanostructures, spheres, cubes, triangles and rods, suspended in water: (a) EM-field enhancement, (b) spectral response and RI sensitivity; (c) Comparison between gold nanorods composed of different ARs, namely their spectral characteristics and response, RI sensitivity.

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# Mineral identification using Laser Induced Breakdown Spectroscopy mapping

**D. Capela<sup>1,2,\*</sup>, M. F. S. Ferreira<sup>1,2</sup>, A. Lima<sup>3,4</sup>, P. A. S. Jorge<sup>1,2</sup>,  
D. Guimarães<sup>2</sup>, N. A. Silva<sup>2</sup>**

<sup>1</sup> Departamento de Física e Astrofísica, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, Porto, Portugal

<sup>2</sup> INESC TEC, Rua do Campo Alegre, 687, 4150-179 Porto, Portugal.

<sup>3</sup> Departamento de Geociências, Ambiente e Ordenamento do Território, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, Porto, Portugal

<sup>4</sup> ICT – Instituto de Ciências da Terra, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, Porto, Portugal

\*email: diana.f.capela@inesctec.pt

Laser Induced Breakdown Spectroscopy (LIBS) is a technique of chemical analysis with a high potential for geological applications [1]. The capability of performing elemental mapping in rock samples with diverse characteristics, allows to better understand the lithosphere composition, as well as the geological alterations that occur there.

Starting from the elementary maps, we developed a methodology based on clustering machine learning algorithms to analyze the LIBS spectral data, in order to classify the minerals present in different samples. Taking various rock types as case studies, the results suggests that our method provides a reliable way to classify and identify mineral types based on their elemental composition. These findings indicate that LIBS can be a complementary diagnostic tool in geology and mining environments.

## Acknowledgments

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# Temporal characterization of broadband femtosecond laser pulses by surface third-harmonic dispersion scan with ptychographic retrieval

Tiago Gomes<sup>1,2</sup>, Miguel Canhota<sup>1</sup>, Helder Crespo<sup>1,3</sup>

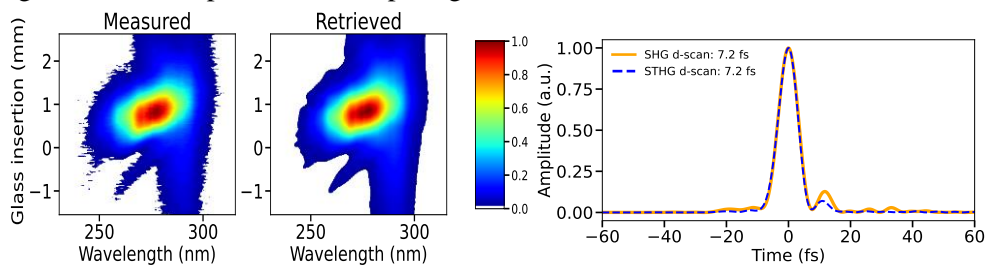
<sup>1</sup> IFIMUP and Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal

email: tdsg2000@hw.ac.uk

<sup>2</sup> The Institute of Photonics and Quantum Sciences, Heriot-Watt University, Edinburgh EH14 4AS, Scotland, UK

<sup>3</sup> Present Address: Blackett Laboratory, Imperial College, London SW7 2AZ, UK

Ultrashort laser pulses have applications in spectroscopy, microfabrication and microscopy. As such pulses cannot be detected solely by electronic devices, they traditionally required complex optical setups for their temporal measurement. Dispersion-scan (d-scan) is a relatively new, simpler, ultrashort pulse characterization technique capable of characterizing the shortest optical laser pulses known to date, in the single-cycle and sub-3-femtosecond regime [1]. In this work, recently accepted for publication in *Optics Letters*, the d-scan technique is extended to the nonlinear process of surface third-harmonic generation (STHG). The STHG effect is present in every material, unlike second-harmonic generation (SHG) that requires non-centrosymmetric materials. Furthermore, STHG-based d-scan is attractive for the characterization of a new generation of laser sources in the mid-infrared region as the generated nonlinear signal lies in the very convenient visible to near-infrared spectral range. Our d-scan setup is further complemented with a ptychographic retrieval algorithm [2], with modifications to accommodate the retrieval of broadband pulses in the few-cycle, few-femtosecond regime. The proposed setup is robust, comprised of readily available materials and, together with the ptychographic algorithm, can faithfully retrieve pulses from low signal-to-noise ratio d-scan traces. We demonstrate the technique by fully characterizing sub-8-fs laser pulses and comparing with standard SHG d-scan.



**Figure 1.** (Left) Measured and retrieved STHG d-scan traces. (Right) Retrieved pulse temporal profiles and comparison with standard SHG d-scan.

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# DEVELOPMENT AND CHARACTERIZATION OF AN ULTRA-BROADBAND 7 FS LASER OSCILLATOR FOR MULTICOLOR NON-LINEAR IMAGING

**Tiago E. C. Magalhães**,<sup>1</sup> **Miguel Miranda**,<sup>2</sup> **Paulo T. Guerreiro**,<sup>2</sup> **Rosa Romero**,<sup>2</sup>  
**Helder Crespo**<sup>1,2</sup>

<sup>1</sup>Instituto de Física de Materiais Avançados, Nanotecnologia e Fotónica (IFIMUP), Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal. email: tecmagalhaes@fc.up.pt

<sup>2</sup>Sphere Ultrafast Photonics, R. do Campo Alegre 1021, Edifício FC6, 4169-007 Porto, Portugal.

Multicolor nonlinear imaging with ultra-broadband 7 femtosecond laser was recently demonstrated [1], where biological samples labeled with different chromophores were simultaneously excited and tracked. In this work, we present a custom-built single-box mode-locked laser oscillator with a built-in compressor to be used in a nonlinear imaging system. The laser cavity design was based on the one described previously in [2]. The spectral bandwidth covers the 630-1040 nm range with a repetition rate of ~80 MHz. The spectrum can be slightly tuned (redshifted and blueshifted) by moving the intracavity wedges, which can be used to enhance regions where chromophores are more efficient. The maximum mode-locked average power measured is 180 mW, corresponding to a pulse energy of 2.25 nJ. This average power can be reduced down to ~90 mW, which can be useful for some samples (e.g., limitations in terms of intensity or long exposure). The compressor inside the box, consisting of chirped mirrors and a pair of wedges, is used for both dispersion control and ultrashort pulse characterization through the d-scan technique [3]. The observed stability of this mode-locked laser demonstrates its capability to operate in nonlinear imaging systems with long-hour scans.

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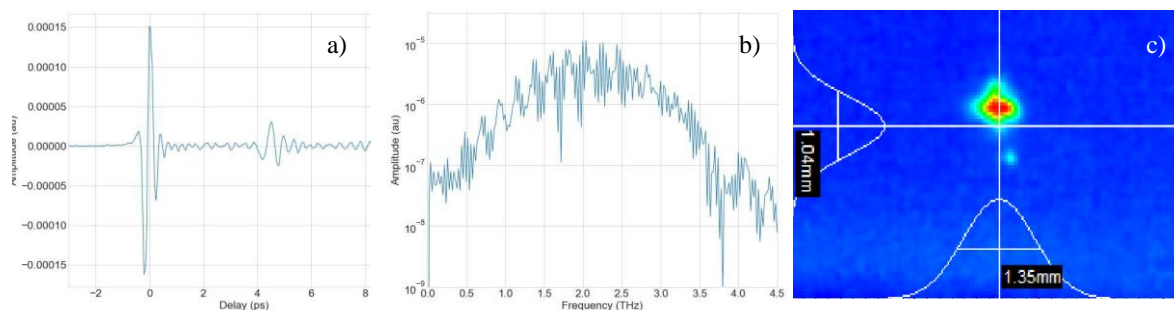
# THz time-domain spectroscopy using a femtosecond laser-plasma source

**Ana Oliveira e Silva<sup>1</sup>, Miguel Canhota<sup>1</sup>, Helder Crespo<sup>1,2</sup>**

<sup>1</sup> IFIMUP and Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal  
email: ana.miguel.o.silva@gmail.com

<sup>2</sup> Present Address: Blackett Laboratory, Imperial College, London SW7 2AZ, UK

Here we present a new broadband, versatile, and optimized THz source and time domain spectrometer. To the best of our knowledge, this is the first THz spectrometer entirely designed and built in Portugal. It uses a femtosecond laser amplifier with 30 fs pulse duration, 1 mJ pulse energy, 1 kHz repetition rate and 800 nm central wavelength. The THz pulses are generated by focusing the fundamental and the second harmonic of the amplifier pulses in air. This two-colour air plasma technique can generate broadband radiation from 0.1 up to 10 THz or more depending on the laser source used [1]. Since we cannot detect the THz field directly using electronic devices, we opted to use a coherent detection technique called electro-optical sampling. In this technique, the THz electric field (ps duration) is sampled with a portion of the original femtosecond laser pulses [2]. After obtaining the THz field directly in the time domain, a FFT is used to retrieve its spectrum – see Figures 1(a) and (b). We also optimized the THz generation by using a fully in-line optical setup to generate the second harmonic pulses, correct the time delay and phase between second harmonic and fundamental pulses, and align the polarization of the fundamental field with the second harmonic one. With this versatile spectrometer one can do measurements of optical parameters such as the complex refractive index, as well as obtain the transmittance of samples or even study phononic excitations of materials in the THz range. The applications are many, ranging from fundamental studies of materials and devices, to sensing and security applications. Currently, we are characterizing this spectrometer by measuring the achieved THz beam energy and spatial profile – see Figure 1(c).



**Figure 1** (a) THz time domain signal and (b) corresponding power spectrum measured at 10% relative humidity. (c) THz spot profile at the focus, measured with a THz camera.

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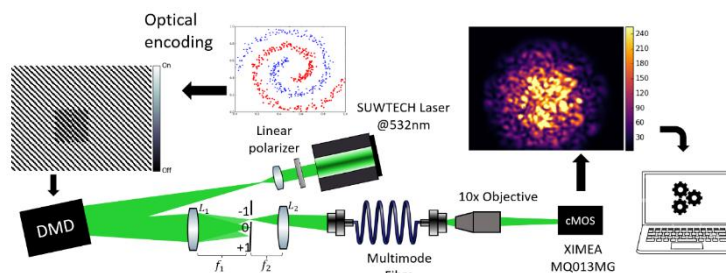
# Taming light for novel computing machines

**Duarte Silva,<sup>1,2</sup> Nuno A. Silva<sup>1,2</sup>, Tiago D. Ferreira<sup>1,2</sup>, Carla C. Rosa<sup>1,2</sup>,  
Ariel Guerreiro<sup>1,2</sup>**

<sup>1</sup>Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal.

<sup>2</sup> INESC TEC, Centre of Applied Photonics, Rua do Campo Alegre 687, 4169-007 Porto, Portugal.  
email: duartejfs@hotmail.com

The performance of neural networks has been found to be intrinsically tied to its scalability. With Moore's law reaching a plateau, emerges the need to continue performance scaling in the absence of electronics miniaturization. A promising route onwards lies within hardware specialization, which is particularly attractive for machine learning applications. Leveraging optics as a workhorse brings natural advantages as compared to electronics, namely its intrinsic parallelism, high bandwidth and low energy consumption. In this work we present an optical implementation of an Extreme Learning Machine (ELM) based on the dynamics of optical complex systems[1], as illustrated in figure 1. In short, ELMs are an artificial intelligence framework based on a network of hidden neurons with random fixed weights and biases, that generate a complex behaviour in response to an input[2]. The values at the output layer can be used to train a linear transformation to solve a particular computational task. We propose and experimentally validate a theoretical model which outlines in detail the effective activation function of each output neuron. On top of that, we have also studied the learning capabilities of our machine in regimes with weak and strong physical non-linearities. Furthermore, the recent success of diffractive optical neural networks demonstrates attractive computational capabilities using only optical linear elements[3], thus we extend our ELM to an all-optical computing device and test it on standard machine learning tasks.



**Figure 1.** Illustration of the optical set-up and methods for an optical ELM.

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# Using fluids of light in photorefractive media to create turbulent states

**Tiago D. Ferreira<sup>1,2</sup>, Nuno A. Silva<sup>1,2</sup>, Duarte Silva<sup>1,2</sup>, Vicente Rocha<sup>1,2</sup>, Carla C. Rosa<sup>1,2</sup>,  
and Ariel Guerreiro<sup>1,2</sup>**

<sup>1</sup>Department of Physics and Astronomy, Faculty of Sciences, University of Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal.

<sup>2</sup>INESC TEC, Centre of Applied Photonics, Rua do Campo Alegre 687, 4169-007 Porto, Portugal  
email: tiagodsferreira@hotmail.com

Both a light beam that propagates through a nonlinear medium and a quantum fluid are described by a similar mathematical model. This analogy has allowed researchers to investigate quantum-like complex dynamics in affordable and faithful two-dimensional experimental setups [1]. Such dynamics span from gravity analogues to superfluid-like flows. Beyond these, fluids of light can also be used to create and study turbulent dynamics, a complex and not fully comprehended behaviour, in a controllable manner [2]. In this work, we use a photorefractive crystal as a nonlinear medium and disturb a fluid of light with an all-optical defect. By varying the relative velocity between the fluid and the defect, we can observe the emission of vortices, which are a hallmark of turbulent dynamics. The reconstruction of the complex representation (amplitude and phase) of the turbulent state, using a holographic technique, allows examining the presence of energy cascades in the incompressible component of the kinetic energy. These energy cascades are a signature of turbulent states [3] and may be explored and studied in a controllable manner using our setup. The experimental results are compared with numerical simulations.

## Acknowledgements

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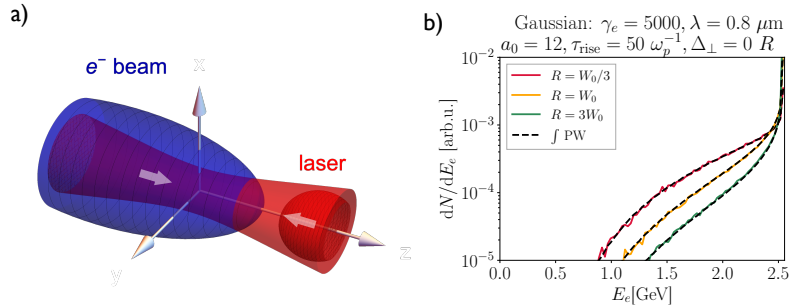
# MODELLING THE FINAL ELECTRON SPECTRA AFTER RADIATION REACTION FROM INTENSE LASER SCATTERING

Óscar Amaro,<sup>1</sup> Marija Vranic<sup>1</sup>

<sup>1</sup>GoLP/Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal  
email: oscar.amaro@tecnico.ulisboa.pt

Upcoming experiments combining state-of-the-art lasers and relativistic electrons will allow a more in-depth understanding of the energy loss mechanisms of electrons in the presence of intense electromagnetic fields, also known as radiation reaction. While several studies have addressed this issue in an idealized setting of point-like electron-beams scattering against Plane Waves, few analytical models have been developed for the collision of arbitrary beam geometries with focused laser pulses (Fig.1 a). In this case, not all electrons will interact with the same peak laser field due to spatio-temporal synchronization effects. However, it is possible to estimate the effective laser intensity of interaction for each fraction of the electron ensemble. This allows the generalization of scaling laws previously derived in the context of a Plane Wave setup to more realistic geometries including 3D effects. Recently, we have shown that the positron yield in focused laser-electron scattering can indeed be computed through this approach [1].

In this work, we have developed a semi-analytical model to estimate the final particle distribution functions, including several non-ideal features, and using either Classical or Quantum Radiation Reaction descriptions. We have demonstrated that it is possible to reconstruct the final electron spectrum in 3D scattering geometries by linearly combining several datasets from 1D Plane Wave simulations (Fig.1 b), thus reducing the dimensionality of the problem. This model has been compiled into a toolkit that may be used to support near-future experiments, namely when searching for signatures from a specific model of Radiation Reaction.



**Figure 1. a)** Scattering of a relativistic electron beam with a focused, intense laser pulse. **b)** Final electron spectra (initially monoenergetic) after collision with laser pulse for various geometries: color – quasi-3D PIC simulations, dashed – reconstructed spectrum from 1D PIC simulation data.

## Acknowledgements

Work with support from FCT grants CEECIND/01906/2018 and PTDC/FIS-PLA/3800/2021.

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# ULTRAFAST OPTICAL PUMP-PROBE SPECTROSCOPY SYSTEM FOR THE STUDY OF PHOTOPHYSICAL PROCESSES IN NANOMATERIALS

**Tânia M. Ribeiro**,<sup>1</sup> **Tiago E. C. Magalhães**,<sup>1</sup> **Helder Crespo**<sup>1,2</sup>

<sup>1</sup>Instituto de Física de Materiais Avançados, Nanotecnologia e Fotónica (IFIMUP), Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal

<sup>2</sup>Present address: Blackett Laboratory, Imperial College, London SW7 2AZ, UK

email: tania.ribeiro@fc.up.pt

Molecular vibrations, photon absorption and emission, and several scattering phenomena are examples of events taking place on timescales ranging from tens of femtoseconds ( $1 \text{ fs} = 10^{-15} \text{ s}$ ) to a few picoseconds ( $1 \text{ ps} = 10^{-12} \text{ s}$ ). To follow these events, a temporal resolution smaller or of the order of the time scale of the process is required. Thanks to advances in ultrafast laser technology, short light pulses can be used to induce and monitor dynamical processes in matter. Pump-probe spectroscopy is an ultrafast time-resolved optical experiment that uses a so-called “probe” laser pulse to indirectly visualize the state of a process [1]. This technique has important applications in optoelectronics, where the development of devices such as high-speed photodetectors relies on the relaxation dynamics of photoexcited charge carriers in the material of interest [2].

Here we present a custom-built degenerate pump-probe setup operating with an ultrafast Ti:Sapphire laser amplifier (Coherent Astrella) delivering  $<35 \text{ fs}$  pulses with an energy of approximately  $7 \text{ mJ}$  at a repetition rate of  $1 \text{ kHz}$ . The principles and applications of pump-probe spectroscopy will be addressed as well as the results obtained with this system for several material samples (e.g., excited carrier lifetime measurements in multilayer graphene films).

## Acknowledgements

Tânia M. Ribeiro acknowledges the support from the Fundação para a Ciência e a Tecnologia (FCT, Portugal) through grant PD/BD/140872/2018. This work was supported by FCT grants PTDC/FIS-OTI/32213/2017 and UIDB/04968/2020), and by the Programa Operacional Temático Factores de Competitividade (NORTE-01-0145-FEDER-022096).

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# Ultrafast Magnetization Dynamics in CoFeB-based Multilayer Thin Films Down to the Few-cycle Regime

**A. S. Silva<sup>1\*</sup>, T. Ferreira<sup>1</sup>, S. P. Sá<sup>1</sup>, S. A. Bunyaev<sup>1</sup>, G. N. Kakazei<sup>1</sup>, M. Canhota<sup>1</sup>, M. Miranda<sup>1</sup>, C. Garcia<sup>2</sup>, I. J. Sola<sup>3</sup>, D. Navas<sup>4</sup> and H. Crespo<sup>1</sup>**

<sup>1</sup>IFIMUP/Dep. de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, 4169-007 Porto, Portugal

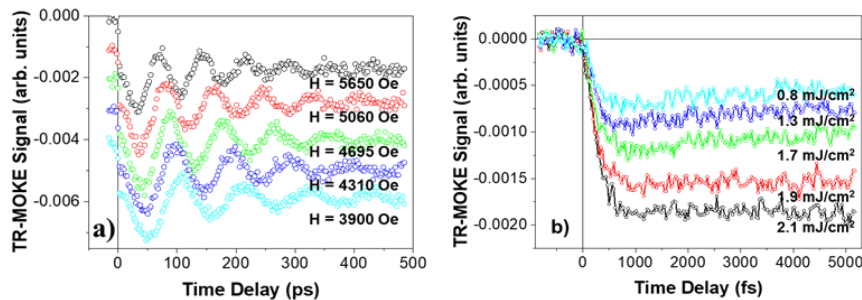
<sup>2</sup>Dep. de Física y CCTVal, Universidad Técnica Federico Santa María, 2390123 Valparaíso, Chile

<sup>3</sup>ALF-USAL, Applied Physics Department, University of Salamanca, E-37008 Salamanca, Spain

<sup>4</sup>Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC, 28049 Madrid, Spain

\*anasilva@fc.up.pt

Since Beaurepaire *et al.* in 1996 demonstrated the possibility to manipulate the magnetization using femtosecond (fs) laser pulses [1], time-resolved pump-probe measurements based on the magneto-optical effects have provided an invaluable tool for the study of ultrafast magnetic dynamics in many relevant systems [2]. Although rapid advances in ultrafast optical methods have allowed the temporal resolution to be gradually improved, the measurements are routinely performed with few tens of fs (e.g., 30 - 50 fs). However, achieving an even higher temporal resolution is very important for studying ultrafast processes in matter, such as the spin-orbit coupling, the exchange interaction and the structural anisotropy of the materials, among others. With this in mind, we have developed a unique, compact and versatile time-resolved magneto-optical (TR-MO) system to study ultrafast magnetodynamic processes. Our setup uses state-of-the-art ultrafast optical methods to deliver few-cycle, sub-5-fs, carrier-envelope phase (CEP) stable pump and probe laser pulses at the sample position, permitting the observation of ultrafast magnetization dynamics at unprecedented temporal resolutions in the optical range. The few-cycle regime is also highly promising for the direct excitation and observation of coherent ultrafast magnetodynamic behaviour [3]. Using our TR-MO system, we have performed magnetization dynamics measurements of CoFeB-based multilayer thin films with perpendicular magnetic anisotropy in different temporal regimes, where we were able to track down processes such as precessional motion [4] and ultrafast demagnetization (Figure 1).



**Figure 1.** TR-MOKE measurements on the [CoFeB (3 Å) / Pd (10 Å)]<sub>5</sub> multilayer ultrathin films (a) with different applied magnetic fields and (b) ultrafast demagnetization curves for different laser fluences.

## Acknowledgements

Fundação para a Ciência e a Tecnologia e COMPETE 2020 (FEDER) (POCI-01-0145-FEDER-031302, PTDC/FIS-OTI/32213/2017, UIDB/04968/2020); Programa Operacional Temático Factores de Competitividade (NORTE-01-0145-FEDER-022096).

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## Física dos Plasmas

# SIMULATING FAST PARTICLE CONFINEMENT FOR NEW STELLARATOR CONFIGURATIONS

**Clara Cottet<sup>\*,1</sup>, Rogério Jorge<sup>1</sup>, Paulo Rodrigues<sup>1</sup>, Christopher Smiet<sup>2</sup>**

<sup>1</sup> Instituto Superior Tecnico, 1 Avenida Rovisco Pais, 1049-001 Lisboa

\*email: [claracottet@gmail.com](mailto:claracottet@gmail.com)

<sup>2</sup> Renaissance Fusion, 22 Rue Jean Pierre Timbaud, 38600 Fontaine, France

Good confinement of fast particles is a critical requirement for any nuclear fusion reactor for energy production. In particular, the alpha particles produced in the core by fusion reactions must be confined for long enough to provide heating in order to sustain the burning plasma. Furthermore, localised losses of energetic alpha particles, with a birth energy of 3.5MeV for D-T reactions, can cause damage to the in-vessel components. In tokamaks, the inherent symmetry guarantees the confinement of alpha particles. This is not necessarily true in stellarators due to their complex shape, but can be achieved, for instance by exploiting a property called quasi-symmetry [1]. In this project, the quality of alpha particle confinement is assessed for several new quasi-isodynamic stellarator configurations, with three and four period symmetry, low aspect ratio and finite plasma pressure, that were obtained by optimising for higher rotational transform and minimising the effective ripple. These configurations were provided by Renaissance Fusion, a fusion start-up that is developing designs for a stellarator power-plant, with novel high temperature superconductor coil manufacturing techniques and liquid metal walls. Among other benefits, flowing liquid walls lessen the damage caused by fast particle losses. The large ensemble of alpha particles, launched isotropically on the inner magnetic flux surfaces, constitutes a complex system, where the equations of motion of each particle are evolved to predict their trajectories in the magnetic equilibrium field. The particles' guiding-centre orbits were tracked over their slowing down time using the SIMPLE (Symplectic Integration Methods for Particle Loss Estimation) code [2], that adopts a symplectic integration method in canonical coordinates, and classifies orbits as chaotic or regular for faster computation. The orbits were also traced using the gyronimo code for comparison. Additionally, we explore whether particles initialized with certain magnetic moments, pitch angles and starting point are more likely to be lost, and map the spatial distribution of lost particles to locate any hotspots. Understanding the parameters that lead to improved particle confinement can then be used to update the cost function and feedback into the optimization loop.

## Acknowledgements

Work with support from the Institute of Physics (IOP) and Instituto de Plasmas e Fusão Nuclear (IPFN).

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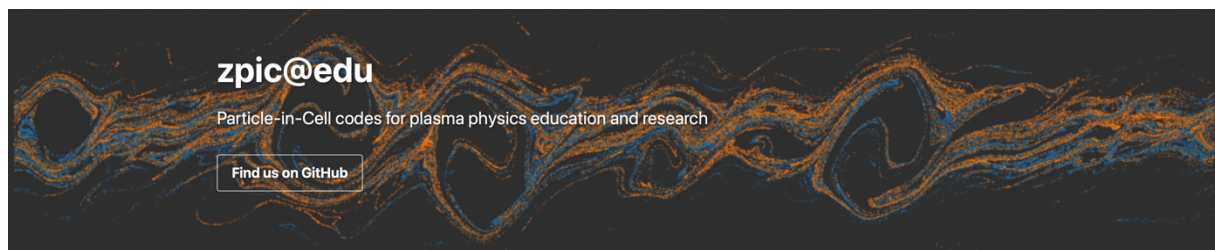
# Plasma physics education using ZPIC

**B. Malaca<sup>1</sup>, M. Pardal<sup>1</sup>, J. Vieira<sup>1</sup>, R. A. Fonseca<sup>1,2</sup>**

<sup>1</sup> GoLP/IPFN - Instituto de Plasmas e Fusão Nuclear, Universidade de Lisboa, Lisboa, Portugal  
email: miguel.j.pardal@tecnico.ulisboa.pt

<sup>2</sup> ISCTE - Instituto Universitário de Lisboa, Lisboa, Portugal

Particle-in-Cell (PIC) codes are used in almost all areas of plasma physics, such as fusion energy research, plasma accelerators, space physics, ion propulsion, and plasma processing, and many other areas. The ZPIC educational code suite [1], that we develop, intends to foster training in plasma physics using computer simulations by providing an easy to access and use framework, that students and researchers can use not only to learn about PIC simulations, but also to explore both textbook and advanced plasma physics scenarios, and to reproduce published results. In this work we present the recent developments of the ZPIC suite, that improve the support for Jupyter (Python) notebooks as way to control and analyze ZPIC simulations. Leveraging on this work, we have prepared a set of well documented notebooks, with example problems of textbook and advanced plasma mechanisms, ranging from Debye shielding, to EM waves in density ramps and kinetic instabilities, that also include instructions for parameter space exploration. Additionally, we also prepared notebooks that reproduce and extend the work done in seminal plasma physics papers, such as the “Laser Electron Accelerator” [2], also allowing for parameter exploration. We also invite contributions to this repository of test problems that will be made freely available to the community provided the notebooks comply with the format defined by the ZPIC team.



**Figure 1.** Snapshot of the official ZPIC documentation website at <https://ricardo-fonseca.github.io/zpic/>. The image on the background shows the results of a simulation of the Two-stream Instability.

## Acknowledgements

## References

[1] The code suite is freely available and hosted on GitHub at:

<https://github.com/ricardo-fonseca/zpic>

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# Modelling a hollow cathode discharge for several noble gases

**Eduardo M. Calvo,<sup>1</sup> Mário J. Pinheiro,<sup>2</sup> Paulo A. Sá<sup>1</sup>**

**1** Centro de Estudos de Fenómenos de Transporte e Departamento de Engenharia Física, Faculdade de Engenharia da Universidade do Porto, Rua Doutor Roberto Frias s/n, 4200-465 Porto, Portugal

**2** Departamento de Física, Instituto Superior Técnico-IST, Universidade de Lisboa, Avenida Rovisco Pais, 1049-001 Lisboa, Portugal

Hall thrusters are widely used in space propulsion as they are very efficient and competitive EP devices, making them outstanding candidates for various applications that encompass small and large satellites, Earth orbit, and interplanetary missions. To maintain the cross-field discharge characteristic of this device, a source of electrons must be present. This is accomplished by introducing an external hollow cathode device near the hall discharge chamber [1].

Usually, a hollow cathode is formed by a refractory tube; an insert that acts as an active electron emitter with low work function, a heater, a downstream plate, and an anode keeper—the temperature increases by wrapping coils (heater), starting the discharge. Finally, the electric field accelerates the emitted electrons towards the high voltage anode [2].

In this work, we proposed a two-dimensional self-consistent model for the hollow cathode discharge to understand the behavior of several propellant noble gases (helium, neon, argon, krypton, and xenon) under the same operating conditions. This simulation used the magnetic field, heat transfer in fluids and solids, laminar flow, and plasma submodules from the COMSOL Multiphysics software.

The magnetic circuit was designed by applying a current of 300A through the wrapped coils; the electric circuit consisted of an anode keeper with 300V and a high-voltage anode with 700V. Finally, the initial and output pressures were used 1Torr and 0Torr, respectively.

## Acknowledgements

We thank the support of FEUP's *Centro de Estudos de Fenómenos de Transporte* for the computational facilities and the financial support.

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**Física Médica e para a Ciência da Vida**

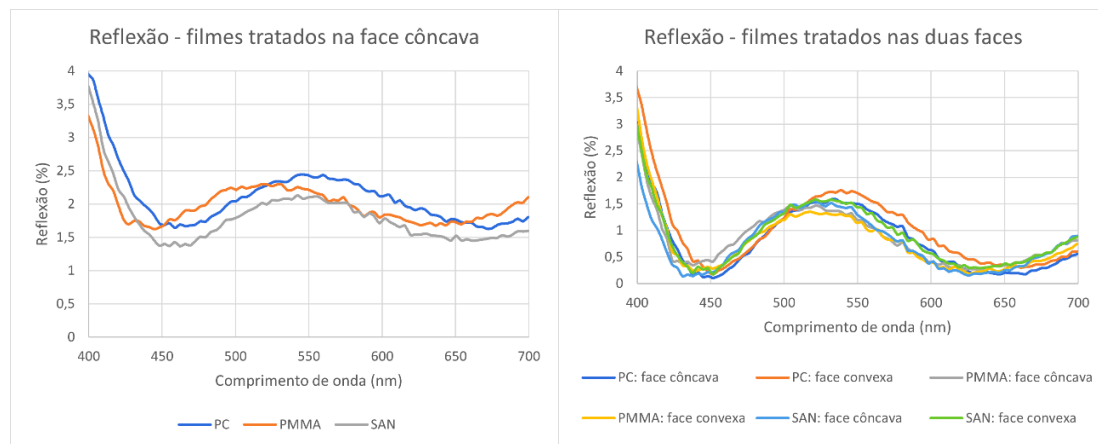
# Revestimentos funcionais para aplicações óticas e oftálmicas

Silvana Guedes<sup>1</sup>, M. Duarte Naia<sup>1,2</sup>

<sup>1</sup>ECT/UTAD - School of Science and Technology, University of Trás-os-Montes e Alto Douro, Vila Real, Portugal. email: silvanacabo\_guedes@hotmail.com; duarte@utad.pt

<sup>2</sup>CEMPRE, Centre for Mechanical Engineering, Materials and Processes, Coimbra, Portugal

Atualmente os revestimentos com filmes finos são utilizados numa grande variedade de aplicações tecnológicas e industriais, desde revestimentos antirreflexo (AR) em lentes oftálmicas, ecrãs táteis e revestimentos de dispositivos médicos [1]. Nos últimos anos os avanços na eletrónica vestível não se têm focado apenas na integração de dispositivos em têxteis, calçado ou acessórios, mas sim em dispositivos em contacto com o corpo humano, como as designadas lentes de contacto inteligentes ou novas plataformas para lentes oculares multifuncionais, por exemplo a distribuição de fármacos. A morfologia, estabilidade e desempenho dos filmes são determinadas pelas técnicas de deposição utilizadas, tornando-se assim importante conseguir uma boa caracterização dos mesmos através da microscopia eletrónica, e das respetivas propriedades óticas por meio da espectroscopia em transmissão e em reflexão [2]. Com a ajuda técnica e métodos numéricos para avaliar e prever as propriedades óticas de filmes mono e multicamada, este trabalho apresenta os resultados da caracterização de revestimentos funcionais utilizados em lentes oftálmicas comerciais e mostra a ferramenta desenvolvida, com auxílio da plataforma de simulação COMSOL Multiphysics [3], para melhorar o controlo e fabrico desses revestimentos. Paralelamente será simulado e desenvolvido o plano de fabrico de uma de nova geração de filmes funcionais para ecrãs táteis.



**Fig. 1-** Espectro de reflexão dos filmes AR em substratos de Policarbonato (PC), Polimetilacrilato de metilo (PMMA) e Copolímero de estireno e acrilonitrilo (SAN) tratados numa face e nas duas faces.

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# Surface functionalization of spin-vortex nano-discs for magneto-mechanically induced damage applications

R. Magalhães<sup>1</sup>; S. Caspani<sup>1</sup>; D. Navas<sup>2</sup>; C. Redondo<sup>3</sup>; R. Morales<sup>3</sup>; S. Lima<sup>4</sup>; S. Reis<sup>4</sup>; C. Nunes<sup>4</sup>; J. P. Araujo<sup>1</sup>; C. T. Sousa<sup>1</sup>

<sup>1</sup> IIFIMUP and DFA Faculdade de Ciências da Universidade do Porto, Porto, Portugal.

<sup>2</sup> Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC, Madrid, Spain.

<sup>3</sup> Dpto. de Química-Física, Universidad del País Vasco UPV/EHU, Bilbao, Spain.

<sup>4</sup> LAQV, REQUIMTE, Faculty of Pharmacy of Porto University, Porto, Portugal.

Novel magnetic nanostructures (MNS) have unique spin arrangements in the ground state, namely a spin-vortex state or a synthetic antiferromagnetic state. These nanomaterials have showed promising results in cell separation and manipulation, as contrast enhancing agents in magnetic resonance imaging, and in magneto-mechanically induced cell annihilation. This last biomedical application requires weaker magnetic fields with lower frequencies, as well as lower concentration of particles, to induce cell death, when compared to magnetic hyperthermia [1,2]. In this work, we developed one subset of biocompatible magnetic nanostructures that exhibit a spin-vortex ground state. First, the mumax3 software was used to perform micromagnetic simulations of sub-micron iron discs, for different interdot distances and aspect-ratios (diameter/thickness) [3]. We found that discs with an aspect ratio between 5 and 15 should sustain the vortex state in remanence [4].

Considering these results, iron nano-discs, with a spin-vortex ground state and about 500 nm in diameter, were fabricated by thermal evaporation on Si substrates pre-patterned by interference lithography. Then, the magnetic vortex nano-discs were released from the substrate by chemical etching of an Al sacrificial layer. Subsequently, cell viability and uptake assays were performed using a human leukaemia monocyte cell line (THP-1) [5]. Several concentrations of non-functionalized and polyethylene glycol (PEG)-functionalized nano-discs were studied by flow cytometry. The aim of this functionalization was to prevent the nano-discs uptake by the cells of the immune system and, therefore, increase their circulation time inside the body. As a result, in both cases, the discs were internalized by the cells and found to be innocuous to them. Additionally, it was observed that the PEG-functionalized nano-discs were internalized in a lower degree.

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# HEMODINÂMICA NA BIFURCAÇÃO DA ARTÉRIA AORTA ABDOMINAL COM UM MODELO DE DUAS FASES

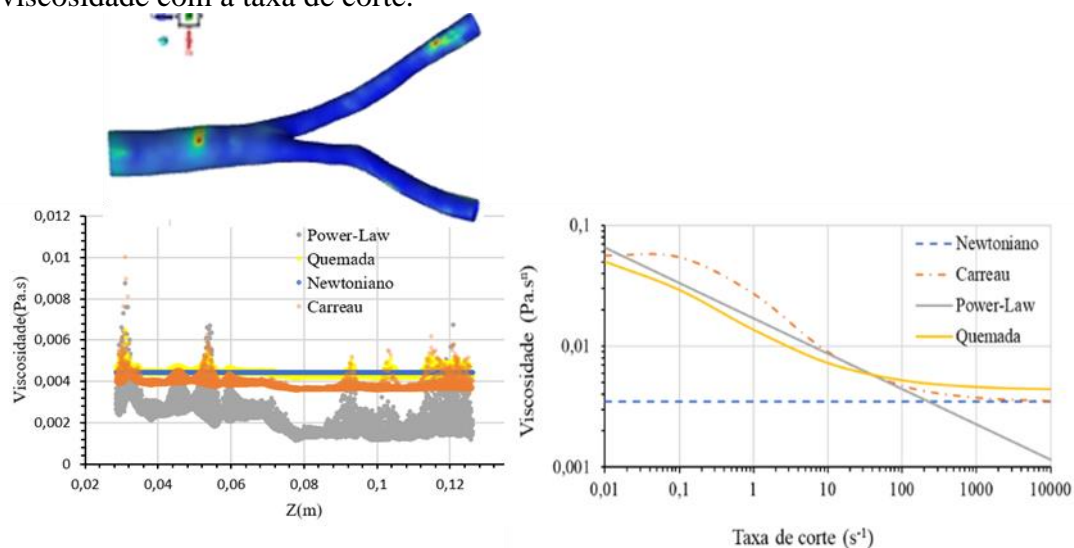
Daniela O. Trigo<sup>1</sup>, Armando A. Soares<sup>1,2</sup>, M. Duarte Naia<sup>1,3</sup>

<sup>1</sup>ECT/UTAD - School of Science and Technology, University of Trás-os-Montes e Alto Douro, Vila Real, Portugal. email: dtrigo1999@hotmail.com; asoares@utad.pt; duarte@utad.pt

<sup>2</sup>EES-INEGI/LAETA, Institute of Science and Innovation in Mechanical and Industrial Engineering, Porto, Portugal.

<sup>3</sup>CEMMPRE, Centre for Mechanical Engineering, Materials and Processes, Coimbra, Portugal.

Este estudo tem como principal objetivo simular o escoamento sanguíneo na bifurcação da artéria aorta abdominal usando um modelo bifásico (plasma e eritrócitos). Para a viscosidade do sangue foram comparados os modelos de viscosidade; newtoniano e não-newtonianos, com o objetivo de compreender a influência da escolha do modelo da viscosidade no comportamento hemodinâmico [1-3]. Com este estudo pretende-se também compreender o comportamento não-newtoniano (Carreau, Power-Law e Quemada) do sangue relativamente ao comportamento newtoniano. Na figura 1, a imagem da artéria mostra para o modelo Power-Law, a distribuição da viscosidade do plasma junto das paredes da artéria (as regiões a vermelho correspondem às regiões onde os valores da viscosidade são mais elevados e a azul onde os valores da viscosidade são mais baixos). Os gráficos de dispersão mostram para os quatro modelos da viscosidade as distribuições da viscosidade ao longo da artéria (eixo dos Z) e o comportamento da viscosidade com a taxa de corte.



**Figura 1-** Distribuição da viscosidade do plasma ao longo da artéria (eixo dos Z) para os modelos de viscosidade: newtoniano, Carreau, Power-Law e Quemada. A imagem da artéria mostra a distribuição da viscosidade nas paredes da artéria quando usamos o modelo Power-Law. O gráfico da direita mostra o comportamento da viscosidade para cada um dos modelos usados.

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# WOUND OPENING IN A THIN INCOMPRESSIBLE VISCOELASTIC TISSUE

G. M. Carvalho<sup>1,2,3</sup>, N. A. M. Araújo<sup>1,2</sup>, P. Patrício<sup>1,4</sup>

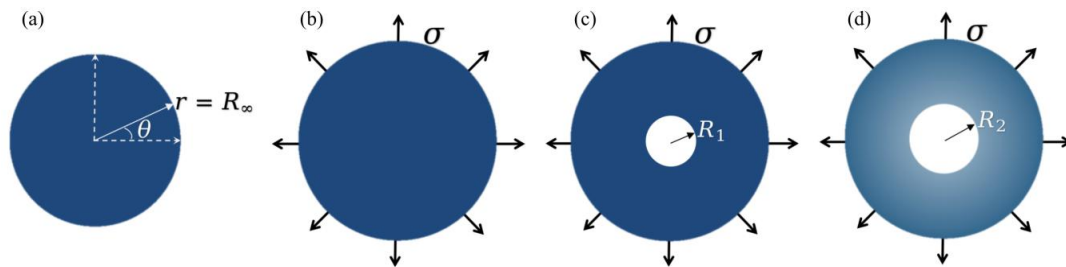
<sup>1</sup>Centro de Física Teórica e Computacional, Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal  
email: gmcarvalho@fc.ul.pt

<sup>2</sup>Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal

<sup>3</sup>Instituto Federal de Educação, Ciência e Tecnologia Catarinense, São Bento do Sul, Brasil

<sup>4</sup>Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, Lisboa, Portugal

Wound healing is essential for the recovery of living organisms. Therefore, it is necessary to better understand how the wound healing process occurs. Recent advances in experimental techniques allow to access the mechanical properties of tissues and monitor their dynamics in real time, opening the possibility of studying the healing process in a systematic way [1, 2]. Along with the development of experimental techniques, it is necessary to develop theoretical models to obtain insight into the biochemical and biophysical processes involved in tissue regeneration [3]. Here, inspired by recent experimental results [4], we develop a model to investigate analytically and numerically the mechanics of wound opening made in a viscoelastic, isotropic, homogeneous, and incompressible thin tissue. Friction between the tissue and its surroundings was also considered. Figure 1 shows how the tissue relaxes after the wound infliction. We find two deformation regimes defined by a single non-dimensional parameter  $\lambda$ , which characterizes the relative importance of viscosity over friction [5].



**Figure 1.** (a) A thin circular tissue of radius  $R_\infty$  at rest. (b) Tissue under a uniform radial distribution of forces, where  $\sigma$  is the force per unit area, applied at the tissue edge, keeping it stretched. (c) The tissue under a uniform radial tension, just immediately after a circular wound of radius  $R_1$ . (d) Final tissue deformation, after relaxation, with a new wound radius,  $R_2$ . The colors gradation reflects the intensity of the tissue radial tension [5].

## Acknowledgements

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# VOLUMETRIC INTERFEROMETRIC LATTICE LIGHT-SHEET IMAGING

**Simao Coelho<sup>1,2,\*</sup>, Bin Cao<sup>2</sup>, Jieru Li<sup>2</sup>, Guanshi Wang<sup>2</sup>, Alexandros Pertsinidis<sup>2</sup>, Ricardo Henriques<sup>1,3,\*</sup>**

<sup>1</sup>Optical Cell Biology, Instituto Gulbenkian de Ciência, Oeiras, 2780-156 Portugal

<sup>2</sup>Structural Biology Program, Memorial Sloan Kettering Cancer Center, NY, USA

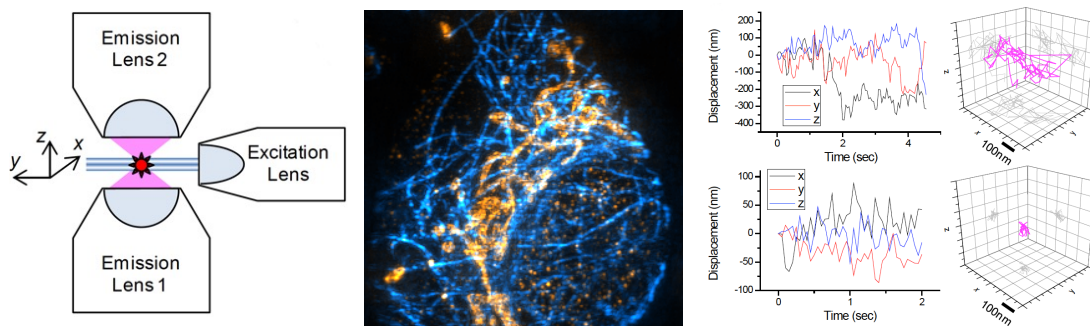
<sup>3</sup>MRC-Laboratory for Molecular Cell Biology, University College London, London, UK

\*Email: [spcoelho@igc.gulbenkian.pt](mailto:spcoelho@igc.gulbenkian.pt), [r.henriques@ucl.ac.uk](mailto:r.henriques@ucl.ac.uk)

**KEY WORDS:** Lattice light sheet, 4-PI, 3D, live-cell imaging, super-resolution microscopy

Lattice light sheet (LLS) microscopy (1) is rapidly becoming the tool of choice for fluorescence light sheet microscopy. LLS microscopy exhibits low photo-toxicity, low photo-bleaching and high background suppression.

Here, we present 3D interferometric lattice light-sheet (3D-iLLS) imaging (2), a technique that requires low excitation light levels, provides high background suppression and substantially improved volumetric resolution by combining 4Pi interferometry (3) with selective plane illumination. We illustrate the performance of 3D-iLLS in a range of systems: single messenger RNA molecules, nanoscale assemblies of transcription regulators in the nucleus, the microtubule cytoskeleton and mitochondria organelles. The enhanced 4D resolution and increased signal-to-noise ratio of 3D-iLLS facilitates the analysis of biological processes at the sub-cellular level. Our results establish 3D-iLLS as a versatile technique with improved volumetric imaging of crowded cellular samples. 3D-iLLS increases the axial (z) resolution to ~100-nm FWHM, compared to ~400-nm FWHM using conventional dithered LLS.



*Figure 1. 3D-iLLS. Left: Schematic of the objective assembly. Two emission objectives are placed perpendicular to a lattice light sheet. Middle: Two-color 3D-iLLS-SIM of Microtubules and Mitochondria in Cos-7 cells. Right: single mRNA dynamics in human osteosarcoma cells.*

*Work with support from National Health and Medical Research Council and Fundação para a Ciência e a Tecnologia*

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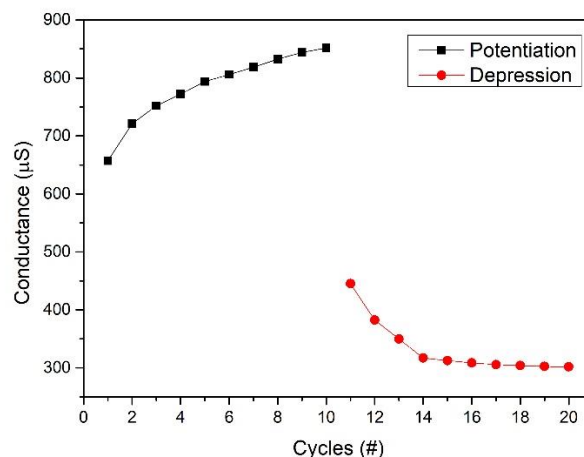
# RESISTIVE-SWITCHING DEVICE BASED ON A COPPER SOLUTION FOR ARTIFICIAL SYNAPSES

Andreia Silva<sup>1\*</sup>, Catarina Dias<sup>1</sup>, João Ventura<sup>1</sup>

<sup>1</sup> IFIMUP, Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Portugal

\*email: up201705822@edu.fc.up.pt

Computer technology has been in fast development for the past decades. However, it might be coming to an end as Moore's law is reaching its limit. Therefore, attention is growing toward neuromorphic computing, that intends to mimic the human brain, the most efficient computational entity known [1]. The brain is composed of a network of neurons and synapses that have the functions of processing and transmitting information, through memory and learning capabilities. A promising solution for the task of mimicking the brain in hardware is a new generation of devices showing resistive switching (RS), a process that resembles the synaptic behavior. In this work a liquid-based resistive-switching two-terminal device was developed. Due to its liquid nature, a great potential for implantable and flexible device purposes is clear, as it can be fabricated in many shapes [2]. A copper active electrode, a platinum inert electrode and a copper(II) sulphate pentahydrate ( $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ ) solution were used. The electrode spacing was varied, different inert electrode materials and solution concentrations were tested, and a temperature study was performed. Low operation voltage was achieved ( $< 300$  mV), with bipolar RS, good endurance and retention. Furthermore, potentiation and depression were achieved, which are believed to be responsible for the learning behavior (see Fig. 1). Lastly, a eutectic liquid composed of choline chloride and glycerol was mixed, revealing that the stability of RS, endurance, retention, potentiation and depression was present and at times improved.



**Figure 1.** Potentiation and depression, represented by the conductance of the device as a function of the cycle of pulses applied.

## Acknowledgements

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# OVERVIEW OF MPGD BASED FULL-FIELD IMAGING SPECTROMETERS – CURRENT STATUS, APPLICATIONS, AND FUTURE DIRECTIONS

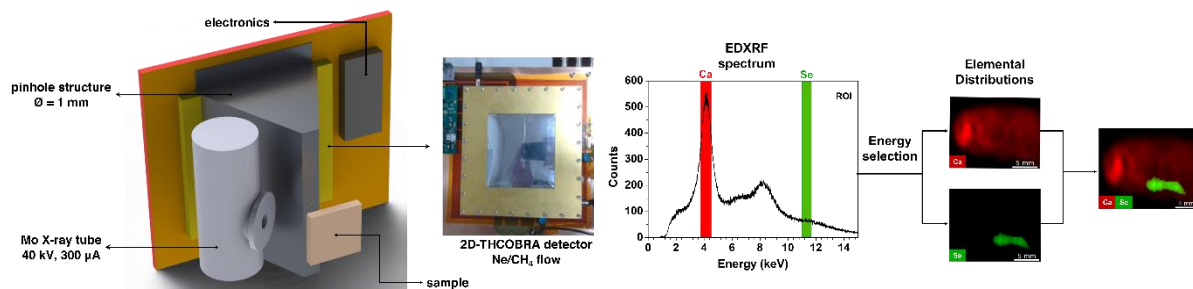
**P. M. S. Carvalho<sup>1</sup>, F. D. Leite<sup>1</sup>, J. F. C. A. Veloso<sup>1</sup>, A. L. M. Silva<sup>1</sup>**

<sup>1</sup>i3N Aveiro, Department of Physics, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro  
email: pmcarvalho@ua.pt

X-ray fluorescence (XRF) techniques are a benchmark for non-destructive elemental analysis in many areas of science and research, from biomedical applications to cultural heritage studies. With XRF, one can obtain quantitative information on the elemental content of samples and map elemental distributions throughout their surfaces. Micro-XRF and Macro-XRF scanning spectrometers are among the most used systems for imaging, but the systems' complexity and high cost precludes its widespread use.

For the past decade, simple and cost-effective full field XRF (FF-XRF) imaging spectrometers based on MicroPattern Gas Detectors (MPGD) have been developed. Such detectors are a very attractive alternative to the more usual semiconductor detectors, as they allow spectral imaging, providing both energy and spatially resolved information, at a fraction of the cost [1].

In this work, we present a FF-XRF system based on the THCOBRA (Fig. 1), a large area ( $10\times 10\text{ cm}^2$ ) MPGD with an energy resolution of  $\sim 1\text{ keV}$  FWHM at 5.9 keV and spatial resolution of  $400\text{ }\mu\text{m}$  [2]. The system's operation and performance are discussed, and practical applications (e.g., heavy metal mapping in Zebrafish – Fig. 1, assessment of ceramic restorations) are presented. Moreover, recent studies concerning the improvement of the system's performance (e.g., implementation of gas purification systems, design of novel optical components) are addressed.



**Figure 1.** (Left) 3D rendering of the FF-XRF spectrometer; and picture of the 2D-THCOBRA detector. (Right) Energy spectrum, and elemental (Ca, Se) distribution maps of a Zebrafish analysed with the FF-XRF spectrometer.

## Acknowledgements

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# SIMULAÇÃO DO TRANSPORTE DA LIPOPROTEÍNA DE BAIXA DENSIDADE NA ARTÉRIA AORTA ABDOMINAL

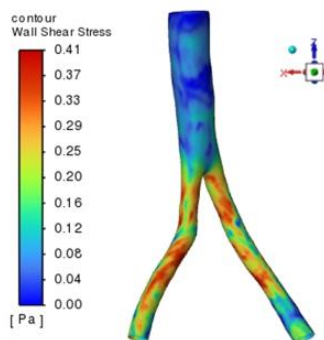
Eliana M. Seixas<sup>1</sup>, Armando A. Soares<sup>1,2</sup>, M. Duarte Naia<sup>1,3</sup>

<sup>1</sup>ECT/UTAD - School of Science and Technology, University of Trás-os-Montes e Alto Douro, Vila Real, Portugal. email: eliana\_seixas3@hotmail.com; asoares@utad.pt; duarte@utad.pt

<sup>2</sup>EES-INEGI/LAETA, Institute of Science and Innovation in Mechanical and Industrial Engineering, Porto, Portugal.

<sup>3</sup>CEMMPRE, Centre for Mechanical Engineering, Materials and Processes, Coimbra, Portugal

O crescimento da placa aterosclerótica leva ao aumento das tensões de corte devido ao escoamento sanguíneo através da secção transversal decrescente do lúmen. Essas tensões de corte podem eventualmente causar a ruptura da placa, resultando na formação de trombos e, eventualmente, num ataque cardíaco. Há muito que se reconhece que a formação da placa aterosclerótica está relacionada com concentração de colesterol no sangue. O principal objetivo deste estudo é compreender a relação entre a hemodinâmica, o transporte e a distribuição de lipoproteínas de baixa densidade (LDL) na artéria aorta abdominal para um paciente específico recorrendo à dinâmica de fluidos computacional. Para a simulação considerou-se um modelo bifásico constituído por sangue (99,88%) e LDL (0,12%). Para a viscosidade sanguínea utilizou-se o modelo não-newtoniano de Carreau. Neste trabalho são investigadas as distribuições das tensões de corte nas paredes da artéria, da velocidade, das taxas de deformação e da concentração de LDL nas paredes da artéria [1-4]. A figura 1 mostra a distribuição da tensão de corte nas paredes da artéria no instante do batimento cardíaco correspondente ao pico sistólico. Neste estudo também se procura compreender como a concentração de LDL influencia a hemodinâmica.



**Figura 1-** Distribuição das tensões de corte nas paredes da artéria no instante correspondente ao pico sistólico.

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# APPLYING MACHINE LEARNING TECHNIQUES FOR QUALITY EVALUATION OF COMPLEX RADIOTHERAPY TREATMENTS

L. Ebrahimpour<sup>1,2\*</sup>, S. Silva<sup>1,2</sup>, D. Pimparel<sup>1,2</sup>, I. Domingues<sup>3,2</sup>, B. Mendes<sup>1,2</sup>, J. Lencart<sup>1,2</sup>, F. Dias<sup>1,2</sup>, J.A.M. Santos<sup>1,2,4</sup>

<sup>1</sup> Medical Physics Service, Portuguese Oncology Institute of Porto (IPOP), Portugal <sup>2</sup> Medical Physics, Radiobiology and Radiation Protection Group, IPO Porto Research Center (CI-IPOP), Porto, Portugal, <sup>3</sup> Politécnico de Coimbra, ISEC, DEIS, Portugal, <sup>4</sup> Instituto de Ciências Biomédicas Abel Salazar (ICBAS), Porto, Portugal. \*L.ebrahimpour@gmail.com

**Introduction:** Medical Physics role in External Beam Radiotherapy (EBR) includes Quality Control (QC) procedures essential to ensure patient safety. However, most procedures are still poorly automated and time consuming. In particular, patient specific quality assurance (PSQA) of a treatment plan (TP) is performed using error prone commercial tools that calculate the control parameter GPR (Gamma Passing Rate). **Purpose:** Investigate the potentialities of regression and classification Machine Learning (ML) estimators in the analysis and verification of EBR TPs and future application of training models as decision methods of TPs approval. **Methodology:** Sets of 5, 10, 15, 20, and 39 most important calculated features selected by two feature selection methods were used to predict the target in the ML process. Each of the 150 employed ML models was optimized by applying a 10-fold cross-validation grid search on the training data (70% of the data) extracted from 696 prostate treatment arcs to predict the values of GPR and from 506 prostate treatment arcs to predict the classes of GPR for the remaining 30% of the data and the best-performing algorithms were recognized. **Results:** Tables 1 and 2 show brief comparisons between our outcome and the results in the literature. Overall, our results identify SVR, NN, and SVC as the best-performing ML models to predict PSQA outcomes with respect to the evaluation metrics listed in the tables. **Conclusions:** The results can aid the decision-making process during plan optimization. Moreover, the accuracy of the predictions is expected to improve further by employing more data and applying more features, namely *radiomic* features extracted from imaging data.

Table 1: Comparison of the studies on ML and Deep Learning applications for PSQA GPR value predictions

Reference	Data size	ML Algorithm	Target	No. of features	MAPE <sup>9</sup>	No. of data with errors<3.5%	Spearman CC <sup>10</sup>
This work	696	DNN <sup>1</sup>	GPR3 <sup>7</sup>	10	0.02	0.89	0.28
This work	696	RF <sup>2</sup>	GPR3	20	0.02	0.89	0.41
This work	696	SVR <sup>3</sup>	GPR3	39	0.02	0.88	0.42
Li et al. (2019) [1]	303	PR <sup>4</sup>	GPR3	54	--	0.90	--
Tomohiro et al. (2019) [2]	600	NN <sup>5</sup>	GPR3	28	--	--	0.57
This work	696	NN	GPR2 <sup>8</sup>	20	0.02	0.82	0.73
Tomohiro et al. (2019) [2]	600	RTA <sup>6</sup>	GPR2	28	--	--	0.58

<sup>1</sup> Deep Neuronal Network <sup>2</sup> Random Forest <sup>3</sup> Support Vector Regression <sup>4</sup> Poisson Regression <sup>5</sup> Neuronal Network <sup>6</sup> Regression Tree Analysis <sup>7</sup> GPR 3%/3mm <sup>8</sup> GPR 2%/2mm <sup>9</sup> Mean Absolute Percentage Error <sup>10</sup> Spearman Correlation Coefficient

Table 2: Comparison of the studies on ML applications for PSQA GPR class predictions

Reference	Data size	ML Algorithm	Target	No. of features	Accuracy Score	AUC <sup>5</sup> Score	FPR <sup>6</sup>
This work	506	SVC <sup>1</sup>	Class of GPR2 <sup>4</sup>	15	0.76	0.80	0.16
This work	506	DT <sup>2</sup> /RF <sup>3</sup>	Class of GPR2	38	0.76	0.81	0.21
Hirashima et al. (2020) [3]	1255	Tree-based	Class of GPR2	502	--	0.83	--

<sup>1</sup> Support Vector Classifier <sup>2</sup> Decision Tree <sup>3</sup> Random Forest <sup>4</sup> GPR 2%/2mm <sup>5</sup> Area Under ROC Curve <sup>6</sup> False Positive Rate

Acknowledgements: Work with support from the project CI-IPOP-134-2020.

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# MCDHF CALCULATIONS OF EMISSION RATES IN RADIONUCLIDES WITH BIOMEDICAL INTEREST

**J. P. Marques<sup>1</sup>, J. Ekman<sup>2</sup>, B. P. E. Tee<sup>3</sup>, R. du Rietz<sup>2,3</sup>, B. Q. Lee<sup>4</sup>, M. S. Pires<sup>1</sup>, P. Jönsson<sup>2</sup>, T. Kibédi<sup>3</sup>, M. Vos<sup>2</sup>, A. E. Stuchbery<sup>3</sup>, J. M. Sampaio<sup>1</sup>**

<sup>1</sup>Laboratório de Instrumentação e Física Experimental de Partículas (LIP) and Faculdade de Ciências, Universidade de Lisboa (FCUL), Portugal

<sup>2</sup>Department of Materials Science and Applied Mathematics, Malmö University, Malmö S-20506, Sweden

<sup>3</sup>Department of Nuclear Physics and Accelerator Applications, Research School of Physics, Australian National University, Canberra, ACT, Australia

<sup>4</sup>GenesisCare, Theranostics, Melbourne, Victoria, Australia

In this work we present decay emission rates for Auger emission radionuclides with medical interest, calculated with the multi-configuration Dirac-Hartree-Fock method [1]. Calculated radiative and radiationless rates are then used in a Monte-Carlo code to generate the atomic deexcitation cascades that follow the creation of an internal hole via electron capture and/or internal conversion and to simulate an Auger spectrum. Transition rates are calculated with the MCDFGME [2] and the GRASP2K/RATIP [3] codes and compared with the 40-50 years old Evaluated Atomic Data Library values (EADL) values that are still used by most programs for microdosimetric calculations. Our calculations show an overall good agreement between them for individual transition probabilities.

In our days, one of the most interesting applications of this kind of calculations is targeted therapy with low energy Auger electrons generated from outer shells in radionuclides, such as <sup>125</sup>I, placed in the vicinity of the cell nucleus. In those conditions, they are very effective to destroy tumor cells, while minimizing the collateral damage to healthy tissues, because of their high linear energy transfer that can cause irreparable complex damage in the cell DNA. Thus, an accurate knowledge of the emission Auger spectra is essential for dosimetry calculations that quantify the biological effectiveness of the radionuclides used. The comparison with the experimental electron emission spectrum of <sup>125</sup>I shows that our calculations can reproduce very well the structure of the K-LL Auger electron peaks and improve the description of the M Auger peaks below 300 eV, features that cannot be explained using EADL data. This gives us confidence that microdosimetry calculations based on the rates calculated here are an improvement on those using EADL rates.

## Acknowledgements

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# Astrofísica, Cosmologia, Física de Altas Energias



# PARAMETRIC DESIGN OF A CROSS DISPERSED ECHELLE SPECTROGRAPH WITH OFF-THE-SHELF COMPONENTS

**Nuno M. Goncalves,<sup>1,2</sup> A. Cabral<sup>1,2</sup>, M. Abreu<sup>1,2</sup>**

<sup>1</sup> Instituto de Astrofísica e Ciências do Espaço, Universidade de Lisboa, Campo Grande, PT1749-016 Lisboa, Portugal

<sup>2</sup> Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Edifício C8, Campo Grande, PT1749-016 Lisbon, Portugal

email: nmgoncalves@fc.ul.pt

High resolution spectroscopy has a fundamental contribution for modern astronomy. Cross dispersed echelle spectrographs (CDES) are the vanguard of ultra and High Resolution (HR) spectroscopy, being the ESPRESSO instrument in the Very Large Telescope, the current state of the art in terms of spectral resolution [1]. Currently, HR CDES designs for high performances are a demanding challenge to build since they are bulky, costly and complex instruments.

Nowadays, due to the standardization and the developments in the fabrication of optical components, it is simple to obtain off-the-shelf high-quality parts. This paves the way for a variety of high-performance optical instruments to be constructed with such off-the-shelf components. This opens the possibility to build an affordable HR spectrograph with a resolution above the ones available in the marketplace with a comparatively smaller cost.

In this work we present the parametric design of a HR CDES with off-the-shelf components, with a focus in the miniaturization of the solution. For that reason, we performed a trade-off analysis of commercially available optical components to understand how to maintain a low cost and a high enough spectral resolution that it can be applied for astronomy science cases. We applied techniques such as the white pupil concept to keep the instrument design simple and compact [2].

The resulting optical design is for a ground-based spectrograph that has a spectral resolution of  $R \approx 10^5$  and a band of (350 – 730) nm. The achievable resolution was heavily influenced by the usage of off-the-shelf components, limiting the optical components sizes and characteristics.

## Acknowledgements

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## **Stellar characterization for the ARIEL space mission**

Andreas W. Neitzel

Departamento de Física e Astronomia, Faculdade de Ciências da Universidade do Porto,  
Rua do Campo Alegre, s/n, 4169-007

Porto, Portugal

Instituto de Astrofísica e Ciências do Espaço, Universidade do Porto, CAUP, Rua das  
Estrelas, 4150-762 Porto, Portugal

With the discovery of various transiting and eclipsing exoplanets, planetary science is taking a step further with the European Space Agency's Atmospheric Remote-sensing Infrared Exoplanet Large-survey (ARIEL). ARIEL's purpose, the first one of its kind, is the study of the chemical compositions and thermal structures of a large sample of known exoplanets. A crucial step towards the characterization of exoplanets however is the accurate and precision determination of the ages and masses of their host stars, which falls under the purview of the ARIEL Stellar Age/Mass/Radius sub-workgroup. These stellar parameters are usually found in the literature in a case-by-case analysis performed by different teams using different methodologies. The field of stellar oscillations, named Asteroseismology, can further constrain the estimation of fundamental stellar parameters. To this aid, satellites such as CoRoT and Kepler have been providing a growing wealth of high-quality stellar oscillation data to work with.

The aim is the combination of asteroseismic data with spectroscopic and photometric data into a pipeline that makes use of Bayesian methods to estimate the ages, masses, radii and other fundamental parameters of stellar targets. PARAM is the pipeline used in this work and it functions by matching a set of observational constraints to a pre-computed grid of stellar evolutionary models.

The result will be a catalog of ages and masses of exoplanet-host stars that can be used as a benchmark for calibrating age in non-seismic targets.

# DEEP LEARNING IN STELLAR DETECTION AND PHOTOMETRY

**Miguel Silva<sup>1</sup>, Paulo Garcia<sup>1</sup>, Koraljka Muzic<sup>2</sup>, Jaime Cardoso<sup>1,3</sup>**

<sup>1</sup>Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, s/n 4200-465 Porto, Portugal  
email: up200805000@fe.up.pt, pgarcia@fe.up.pt

<sup>2</sup>CENTRA, Faculdade de Ciências, Universidade de Lisboa, Ed. C8, Campo Grande, 1749-016, Lisboa, Portugal

<sup>3</sup>INESC TEC, 4200-465 Porto, Portugal, jaime.cardoso@inesctec.pt

Surveys of deep space stellar clusters are conducted with increasingly advanced instruments. However, many of the algorithms used to process the data are now decades-old [1]. This study aims to ascertain whether novel machine learning models (Faster R-CNN) [2] can improve upon the performance of traditional technologies (DAOPHOT) [3] regarding the detection of stellar objects, localization of the star centre of mass and prediction of their flux.

To test the hypothesis that deep learning can improve on current techniques, two testing grounds were developed. The first consisted of synthetically generating images of a stellar cluster and comparing the performance of the developed Faster R-CNN network with DAOPHOT and the known ground-truth. The second applied the models trained on the first step to a real dataset with images of the Collinder 140 stellar cluster, where the ground truth is not known, but where a catalogue produced by professional photometric analysis was available.

Results show that the Faster R-CNN has a superior performance on the synthetic data, with a precision of 93.7% and recall of 63.7%, versus 96.3% and 37.3% for DAOPHOT, i.e., an extra 7139 stars correctly detected over DAOPHOT, of the 27092 available. The performance on localization of the star centres of mass is also superior for the neural network, with an average absolute error of  $0.52 \pm 0.43$  pixels compared with  $0.85 \pm 0.38$  pixels for the classical approach. The flux prediction shows only a slight edge for the Faster R-CNN with an average absolute error of  $1628 \pm 16902$  electrons versus  $1791 \pm 14514$  electrons for DAOPHOT.

On the test dataset comprising real Collinder 140 images, the detection performance is also superior for the Faster R-CNN with 8507 star detections of the 9629 catalogue sources (88.3%), and proposed an extra 26255 stars. DAOPHOT detected 7175 stars (74.5% of the catalogue proposals), predicting an extra 5430 stars (approximately one-fifth of the Faster-RCNN extra predictions). Regarding the stellar astrometric error, DAOPHOT showed a superior performance with an average absolute error to the catalogue position on unsaturated stars of  $0.10 \pm 0.18$  pixels while the Faster R-CNN registered  $0.90 \pm 0.48$  pixels. The difference to the predicted catalogue flux was also smaller for DAOPHOT with an error of  $6412 \pm 64673$  electrons, while the network had  $13355 \pm 97260$  electrons.

These results suggest that the neural network, despite only being trained on synthetic data, already surpasses the performance of the conventional technique regarding source detection of stellar objects in both synthetic and real images. Further developments are still necessary to improve its performance in real images regarding the localization of the star centres and prediction of their flux. These could entail the development of richer training sets and further customization of the network's architecture for this specific task.

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# THE GRAVITY EXPERIMENT AND THE 2020 PHYSICS NOBEL PRIZE

**Garcia, P. J. V.<sup>1</sup>, Amorim, A.<sup>2</sup> & the Gravity Collaboration**

<sup>1</sup>CENTRA/Faculdade de Engenharia da Universidade do Porto, Portugal  
email: pgarcia@fe.up.pt

<sup>2</sup>ENTRA/Faculdade de Ciências da Universidade de Lisboa, Portugal  
email: aamorim@sim.ul.pt

The GRAVITY experiment [1] was instrumental in the award of part of the 2020 Physics Nobel Prize “for the discovery of a supermassive compact object at the centre of our galaxy”. CENTRA is a member of the GRAVITY consortium, and the GRAVITY+ upgrade of the experiment. GRAVITY is the most advanced optical-infrared instrument in a ground-based observatory. It sharpens the light of four giant 8 m telescopes with advanced adaptive optics and combines it interferometrically.

In this communication we will present the key GRAVITY results that lead to the Nobel Prize: a) the detection of gravitational redshift in the light from the S2 star [2]; b) the detection of orbital motions near the innermost stable circular orbit of the compact object from flares [3].

We will conduct a review of achievements since the Nobel, namely: a) follow-up work on the flare orbital motion [4,5]; b) the detection of Schwarzschild precession in the orbit of S2 [6]; c) routine deep imaging of the stars in close orbit around the black hole [7,8]; d) new constraints on the extended mass component inside the S2 apocenter [9]; d) new significance  $\pm 7 \sigma$  of the Schwarzschild precession detection [9].

The detection of many stars in the close environment of the black hole and the new upgrade of the GRAVITY experiment to GRAVITY+ bring renewed hope to detect a star in orbit close enough to probe the black hole's spin.

## Acknowledgements

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# GRAVITY: THE DARK SIDE OF THE FORCE

Cláudio Gomes<sup>1</sup>

<sup>1</sup>Centro de Física das Universidades do Minho e do Porto  
email: claudio.gomes@fc.up.pt

General Relativity stands out as an elegant and compact gravity theory which correctly describes a vast plethora of phenomena. However, there are some problematic issues regarding its high and its low energy regimes. The first one concerns the incompatibility with a fully quantum description of gravity and the presence of singularities, whilst the latter deals with the mysteries of dark matter and dark energy at astrophysical and cosmological scales, which have not been directly observed so far. These two account for the excess of non-luminous mass seen by its gravitational effect at galactic rotation curves and in clusters of galaxies, and for the late time accelerated expansion of the Universe, respectively. Therefore, several alternative gravitational scenarios have been proposed in the literature, while a deeper look into the Standard Model of Particle Physics and its extensions is being explored to explain these dark components of the Cosmos. In this talk, we shall introduce some of the alternative gravity models as well as some particle physics-motivated approaches. Notwithstanding, there are models proposed by researchers from Portugal.

# LARGE SCALE ATOMIC STRUCTURE CALCULATIONS IN KILONOVAE MODELING

**J. M. Sampaio<sup>1</sup>, R. F. Silva<sup>1</sup>, P. Amaro<sup>2</sup>, G. Leck<sup>3</sup>, A. Flörs<sup>3</sup>, G. Martínez-Pinedo<sup>3,4,5</sup>, J. P. Marques<sup>1</sup>**

<sup>1</sup>Laboratório de Instrumentação e Física Experimental de Partículas (LIP) and Faculdade de Ciências, Universidade de Lisboa (FCUL), Portugal

<sup>2</sup>Laboratory for Instrumentation, Biomedical Engineering and Radiation Physics (LIBPhys-UNL), Department of Physics, NOVA School of Science and Technology, NOVA University Lisbon, 2829-516 Caparica, Portugal

<sup>3</sup>GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany

<sup>4</sup>Institut für Kernphysik (Theoriezentrum), Fachbereich Physik, Technische Universität Darmstadt, Schlossgartenstraße 2, 64298 Darmstadt, Germany

<sup>5</sup>Helmholtz Forschungssakademie Hessen für FAIR, GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany

It has long been theoretically established that observable lanthanides and actinides in the universe originate from the  $r$ -process (rapid neutron capture process). However, no individual lanthanides or actinides have been detected in the single reported neutron star merger from spectroscopic observations. This might be due to the lack of atomic data for lanthanides, and much more so for actinides, which poses a significant challenge for spectroscopic modeling of kilonovae [1].

In this work, we will present large-scale computations of atomic structures and radiative properties needed for computing astrophysical opacities for key  $r$ -process elements. Our primary emphasis is placed on lanthanides and actinides, both of which have datasets that are insufficient, if not completely lacking. To do this, we use the Flexible Atomic Code (FAC), which combines a central potential model and a local approximation of the exchange interaction to derive atomic wavefunctions within the RCI approach. We investigate the effect of the accuracy of low-lying levels on the opacity and how this might be improved by changing the average configuration potential model with available data and by including greater degree of correlation.

A sample of results for a few-weakly ionized ions of relevant  $r$ -process elements is presented, for which atomic data and expansion opacities were computed, under conditions compared to those predicted in neutron star merger-induced kilonova emission. We also investigate the influence of level and line density on opacity and how it converges with the introduction of more configurations. We will specifically illustrate the impact of the proposed interaction configuration model on atomic properties and opacities, as well as some extra impacts, such as the impact of shifting various configuration average energies to match available experimental data (if any).

## Acknowledgements

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## Pentaquarks in a Bethe-Salpeter approach

In the past two decades there has been tremendous progress in the theoretical and experimental investigation of multi-quark states, which has expanded our understanding of what a “hadron” is. Experimental evidence suggests that Nature does not only form “conventional” hadrons such as mesons as quark-antiquark states and baryons as three-quark states, but also more exotic combinations such as tetraquarks and pentaquarks. We present results on pentaquark states in QCD obtained with the Bethe-Salpeter formalism in order to describe the observed LHCb states made of light and charm quarks. We solved the two-body equations for the meson-baryon system which couples the relevant channels in the equation. The interaction that binds such meson-baryon molecules is shaped by one-boson exchanges. Solving the equation allows us to determine the masses of the bound states.

# HEAVY BARYON SPECTROSCOPY IN A QUARK-DIQUARK APPROACH

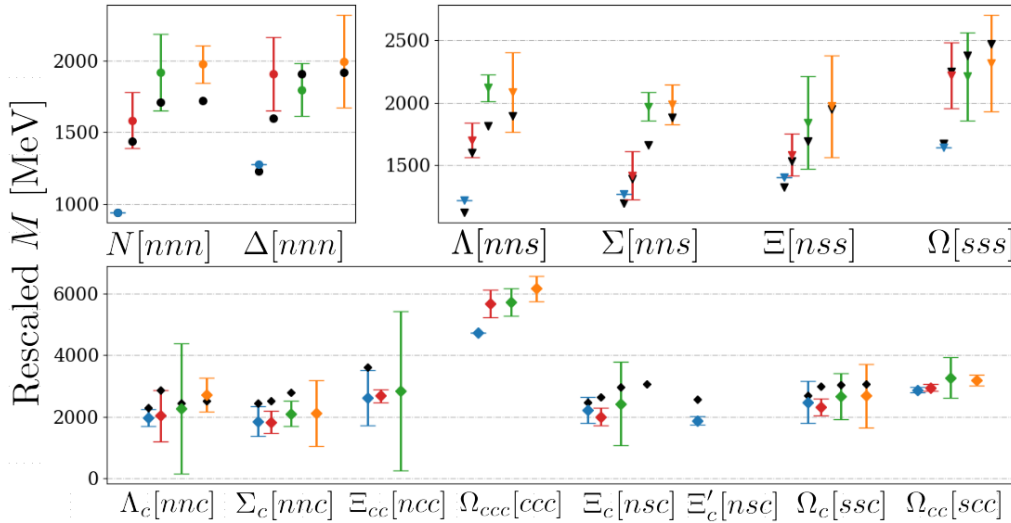
**André Torcato<sup>1</sup>, Gernot Eichmann<sup>2</sup>, Ana Arriaga<sup>3</sup>**

<sup>1</sup>Faculdade de Ciências da Universidade de Lisboa (FCUL), Laboratório de Instrumentação e Física Experimental de Partículas (LIP); email: [atorcato@lip.pt](mailto:atorcato@lip.pt)

<sup>2</sup>Instituto Superior Técnico (IST), Laboratório de Instrumentação e Física Experimental de Partículas (LIP)

<sup>3</sup>Faculdade de Ciências da Universidade de Lisboa (FCUL), Laboratório de Instrumentação e Física Experimental de Partículas (LIP)

We present results for the heavy baryon spectrum for ground and excited states (with positive parity and spins 1/2 and 3/2) using functional methods in Quantum Chromodynamics (QCD). This is the fundamental theory that studies particles constituent of quarks and gluons; baryons are three-quark states and their study can be traced back to Dalitz and its collaborators [1]. We reduce the three-quark Faddeev equations to two-body equations via the quark-diquark approach, where the baryons are treated as bound states of quarks and effective diquarks. The resulting Bethe-Salpeter equation amounts to a quark ping-pong exchange for the interaction kernel, where the quark and diquark ingredients are determined in a rainbow-ladder truncation; a revision of this technique can be found in [2]. Our results show an overall agreement of the ground state masses with experiment. The single charmed baryon ground state masses agree with lattice QCD and theoretical calculations using QCD potential models. A partial wave analysis shows that relativistic effects are present in the baryon amplitude.



**Figure 1.** Our results for the ground (blue), first excited (red), second excited (green) and third excited (yellow) masses of light (upper-left), strange (upper-right) and charmed baryons (bottom). In black, we represent the corresponding experimental states, when available data exists.

## Acknowledgements

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# Going to the light-front with contour deformations

Gernot Eichmann,<sup>1,2,\*</sup> Eduardo Ferreira,<sup>1,2,†</sup> and Alfred Stadler<sup>3,1,2,‡</sup>

<sup>1</sup>*LIP Lisboa, Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal*

<sup>2</sup>*Departamento de Física, Instituto Superior Técnico, 1049-001 Lisboa, Portugal*

<sup>3</sup>*Departamento de Física, Universidade de Évora, 7000-671 Évora, Portugal*

Hadrons are strongly interacting particles composed of quarks and gluons and described by Quantum Chromodynamics (QCD). Their internal structure can be described in terms of structure functions that encode, for example, the momentum and spin distributions of their constituents. Parton distribution functions (PDFs), for example, describe the quark and gluon momentum distributions inside a hadron. These distribution functions are, however, not easy to calculate, because they are defined on the light front, whereas most hadron calculations are performed in a Euclidean metric and yield, for instance, the hadron's Bethe-Salpeter wave functions. The main problem is then to project these Bethe-Salpeter wave functions onto the light front.

We present a new method to compute the light-front wave functions using contour deformations, which we illustrate for a simple system of two interacting scalar particles of equal mass. After solving the two-body Bethe-Salpeter equation, the projection onto the light front is done through a combination of contour deformations and analytic continuation methods. The resulting light-front wave functions and distribution amplitudes are in agreement with the Nakanishi method frequently used in the literature. We show that the contour deformation method can also be used for particles of unequal masses, as well as particles with complex conjugate propagator poles, to make contact with QCD. Finally, we explore ways of extending this method to the calculation of more general parton distributions, such as transverse momentum distributions (TMDs) and generalized parton distributions (GPDs).

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\* gernot.eichmann@tecnico.ulisboa.pt

† eduardo.b.ferreira@tecnico.ulisboa.pt

‡ stadler@uevora.pt

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## **Geofísica, Oceanografia e Meteorologia**

# Potencial migração da adequação bioclimática de diferentes castas de uva portuguesas na Europa devido às alterações climáticas

Filipe J. S. F. Adão<sup>1\*</sup>, João C. Campos<sup>2</sup>, João A. Santos<sup>1</sup>, Aureliano C. Malheiro<sup>1</sup>, Hélder Fraga<sup>1</sup>

<sup>1</sup>*Centre for the Research and Technology of Agro-Environmental and Biological Sciences, CI-TAB, University of Trás-os-Montes e Alto Douro, UTAD, Quinta dos Prados, 5000-801, Vila Real, Portugal*

<sup>2</sup>*CICGE - Centro de Investigação em Ciências Geo-Espaciais, Faculty of Sciences, University of Porto, Alameda do Monte da Virgem, 4430-146 Vila Nova de Gaia, Portugal*

\*Contacto: [filipeadao@utad.pt](mailto:filipeadao@utad.pt)

As alterações climáticas têm impulsionado as tendências de aquecimento e mudanças nos padrões e regimes de precipitação em toda a Europa, que por sua vez têm vindo a afetar a viticultura e a vinificação. Projeções futuras apontam para um reforço das mesmas, e caso se verifique, a sustentabilidade da viticultura no sul da Europa estará em risco. Para melhor compreender como as ditas alterações do clima podem afetar espacialmente a viticultura na Europa, foram desenvolvidos modelos correlativos para aferir a adequação bioclimática de Portugal, Espanha, França e Itália, para doze castas de uva Portuguesas. Os modelos foram produzidos com a plataforma BIOMOD2, utilizando quatro índices bioclimáticos enquanto variáveis preditivas, nomeadamente o índice de Huglin, o índice “Cool Night”, o índice “Growing Season Precipitation” e o índice “Temperature Range during Ripening”. Estes permitiram identificar, para as condições climáticas do passado recente, várias áreas com diferentes graus de adequação bioclimática para as diferentes castas, tanto nos locais onde se encontram atualmente em Portugal e em seu redor, mas também em outras zonas que incluem os restantes países em estudo. Para o futuro, segundo os cenários RCP4.5 e RCP8.5, verificou-se um deslocamento considerável da adequação climática para norte, nomeadamente para o norte de Espanha e França. Em alguns casos, esta deslocou-se também para áreas de maior altitude. Os resultados indicam que a adequação bioclimática das diferentes castas é altamente dependente da temperatura e da precipitação, dado que o deslocamento da mesma segue os padrões de aumento da primeira e de redução da segunda. Medidas adequadas para assegurar a sustentabilidade da viticultura terão necessariamente que mitigar os efeitos de eventuais mudanças destas duas variáveis no futuro.

## Agradecimentos

O trabalho foi apoiado pelo projeto AgrifoodXXI (NORTE-45-2020-20) financiado por Fundos Nacionais pela Fundação Portuguesa para a Ciência e Tecnologia (FCT). Reconhecemos o projeto CoaClimateRisk (COA/CAC/0030/2019) financiado por Fundos Nacionais pela Fundação Portuguesa para a Ciência e a Tecnologia (FCT). Este trabalho foi também apoiado por Fundos Nacionais pela FCT - Fundação Portuguesa para a Ciência e Tecnologia, no âmbito do projeto UIDB/04033/2020.

# CLIMATE IN THE EASTERN BOUNDARY OF THE ATLANTIC

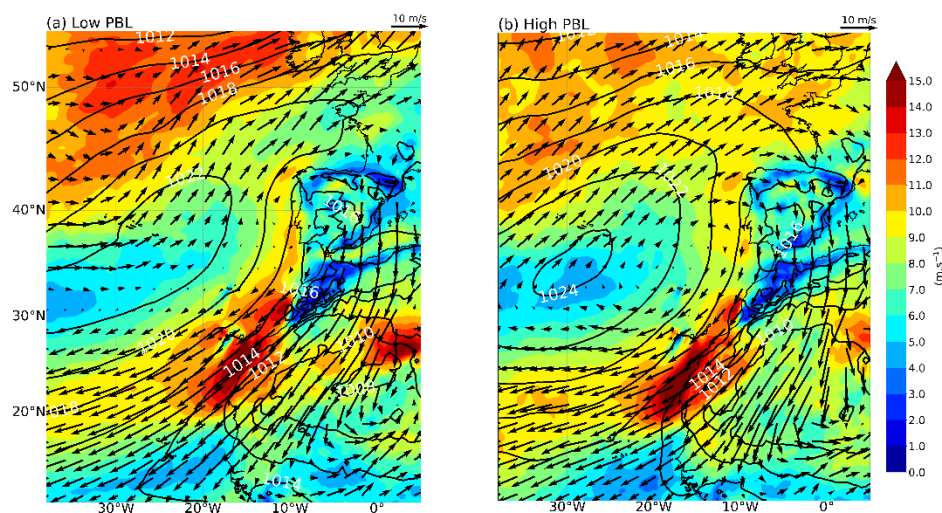
Pedro M. A. Miranda<sup>1</sup>, José Alves<sup>1,2</sup>, Rui Caldeira<sup>1,2</sup>

<sup>1</sup>Instituto Dom Luiz, Faculdade de Ciências, Universidade de Lisboa

email: pmmiranda@fc.ul.pt

<sup>2</sup> Observatório Oceânico da Madeira

Climate in the marine subtropics is largely controlled by the dynamics of the permanent atmospheric anticyclonic systems, such as the Azores anticyclone. In the eastern boundary of the ocean basins, such systems interact with the ocean, and with coastal topography, giving rise to an equatorward cold current maintained by coastal upwelling. Recent studies found evidence of a strong multiweek oscillation in that regional circulation [3], associated with a reshaping of the Azores anticyclone (Figure 1), leading to strong variations of the magnitude of low-level jets near the coast and the islands of Madeira and the Canaries [1,2] and imposing a response from the upper ocean with changes in its temperature and vertical mixing. Because the anticyclone is due to the existence of the Hadley Cell, linking the tropics with the midlatitudes, that variability is relevant in the context of global climate change. The increase in the frequency of strong low-level wind in Madeira airport appears to be part of a multidecadal trend in the NE Atlantic subtropics [3].



**Figure 1.** Sea level pressure (lines), 10m wind speed (color shading), and 10 m wind vectors (arrows) in 2019 summer: (a) low boundary layer at 31N; (b) high boundary layer at 31N.

## Acknowledgements

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# Assessing the future wind energy potential along the Portuguese coast using CMIP6 model ensemble and WRF high resolution simulations

A. Claro<sup>1\*</sup>, J. A. Santos<sup>1\*</sup>, D. Carvalho<sup>2\*</sup>

<sup>1</sup> Physics Department, Centre for the Research and Technology of Agro-Environmental and Biological Sciences, CITAB, Universidade de Trás-os-Montes e Alto Douro, UTAD, 5000-801 Vila Real, Portugal

<sup>2</sup> CESAM - Department of Physics, University of Aveiro, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal

Future wind energy fluxes along the Portuguese coast were estimated under an IPCC future socioeconomic scenario (IPCC SSP5-8.5), for the end (2081-2100) and middle (2046-2065) of the century. The study approach consisted, firstly, in evaluating the large-scale atmospheric circulation changes over the North Atlantic Ocean with kinetic energy (KE) and sea level pressure (SLP) data coming from a CMIP6 multi-model ensemble (described in Table 1). Secondly, wind energy flux and direction were calculated using wind speed data from a WRF 6 km resolution simulation over continental Portugal and nearby Atlantic Ocean. Study results on the WRF simulation data have shown an increase in offshore wind energy flux during Summer (as seen in Figure 1) and a decrease in onshore wind energy flux during Autumn, at the end of the century. The increase during Summer is due to an intensification of the Northern winds, and the decrease during Autumn is caused by the displacement of the jet stream to North.

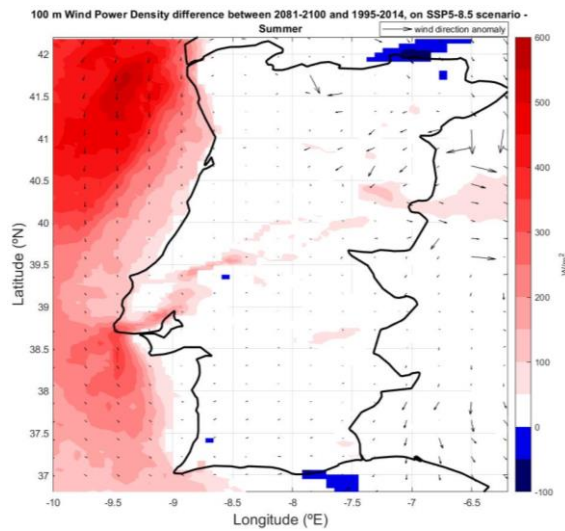


Figure 1: 100 m Wind Energy Flux ( $W/m^2$ ) difference between 2081-2100 and 1995-2014 during Summer, on SSP5-8.5 scenario (WRF simulations). Black arrows represent the wind direction anomaly.

GCM	Institution	Horizontal resolution
CMCC-CM2-SR5	Euro-Mediterranean Centre on Climate Change (CMCC), Italy	1,25° lat x 0,938° lon
CMCC-ESM2		
EC-Earth3	EC-Earth-Consortium (12 European countries)	0,703° lat x 0,703° lon
EC-Earth3-Veg		
MPI-ESM1-2-HR	Max Planck Institute for Meteorology (MPI-M), Germany	0,938° lat x 0,938° lon
MRI-ESM2-0	Meteorological Research Institute (MRI), Japan	1,125° lat x 1,125° lon

Table 1: CMIP6 GCM models used, their horizontal resolution, and the institutions providing them.

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\*E-mail addresses: [andreclaro@ua.pt](mailto:andreclaro@ua.pt) (A. Claro); [jsantos@utad.pt](mailto:jsantos@utad.pt) (J. A. Santos); [david.carvalho@ua.pt](mailto:david.carvalho@ua.pt) (D. Carvalho).



# BIASES IN THE VERTICALLY AVERAGED ATMOSPHERIC CIRCULATION SIMULATED BY CMIP6 MODELS

José M. Castanheira,<sup>1</sup> Carlos A. F. Marques<sup>2</sup>

<sup>1</sup>CESAM & Departamento de Física, Universidade de Aveiro, 3810-193, Aveiro  
email: jcast@ua.pt

<sup>2</sup>CESAM & Departamento de Física, Universidade de Aveiro, 3810-193, Aveiro  
email: cafm@ua.pt

In this communication, we will present results from an analysis of the variability of the vertically averaged (i.e., barotropic) atmospheric circulation simulated by climate models, which integrate the current Coupled Model Intercomparison Project (CMIP6). The variabilities in two ensembles of Atmospheric Model Intercomparison Project (AMIP) simulations were compared with the variabilities in two ensembles of fully coupled simulation counterparts of the current CMIP6 [1].

The atmospheric models simulate less variability of the barotropic atmospheric circulation over the Northern Atlantic and more variability over the North Pacific when compared with the corresponding variabilities in the ERA5 reanalysis (“observations”), at intraseasonal and inter-annual scales. When integrated over the whole globe, the variability in the coupled climate simulations is smaller than the variability in the corresponding AMIP simulations. The smaller global variability of the coupled simulations results in no mean overestimation of the subtropical jet variability in the North Pacific, but further underestimation of the jet stream variability in the Northern Atlantic. The results suggest that the reduction of the biases in the barotropic atmospheric variability over the North Pacific, in the coupled climate simulations, is achieved through compensating biases in the mean Sea Surface Temperatures (SSTs). Moreover, the reduction of the positive biases in the North Pacific seems to be associated with a reduction of the excitation of the most unstable barotropic mode of the atmospheric circulation, which contributes also to a reduction of the barotropic atmospheric variability in the North Atlantic region.

## Acknowledgements

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# LIGHTNING MODELLING IN NUMERICAL WEATHER PREDICTION

**Salgado R<sup>1,2</sup>, Couto FT<sup>1</sup>, Iakunin M<sup>1</sup>, Pinto P<sup>3</sup>, Viegas T<sup>3</sup>, Pinty J-P<sup>4</sup>**

<sup>1</sup> Instituto de Ciências da Terra – ICT (Polo de Évora), Universidade de Évora, Évora, Portugal. rsal@uevora.pt

<sup>2</sup> Departamento de Física, Escola de Ciências e Tecnologia, Universidade de Évora, Évora, Portugal.

<sup>3</sup> Instituto Português do Mar e da Atmosfera (IPMA), Lisbon, Portugal.

<sup>4</sup> Laboratoire d'Aérodynamique, Université de Toulouse, Toulouse, France.

The explicit representation of the atmospheric electric field in numerical weather prediction models is a current challenge. This representation will allow a physically based lightning forecast. Present study aims to assess the performance of the Cloud ELectrification and Lightning Scheme (CELLS) [1] coupled to the Meso-NH atmospheric mesoscale research model [2] in simulating Cloud-to-Ground (CG) flashes. The 17th June 2017 fire events over central Portugal (including the dramatic Pedrogão Grande wildfire) were considered as a real case study. According to an official report of the Portuguese authorities, nine ignition points were reported during that afternoon, some of them caused by lightning.

The study discusses the atmospheric conditions that were favorable to lightning flashes production, as well as the possibility to correctly diagnose cloud-to-ground (CG) flashes using high resolution simulations. The simulation was configured with two nested domains of 4 km and 1 km horizontal resolution (Figure 1) and 50 vertical levels, with the innermost domain centred in the area where forest fires occurred. The description of the electrical state of a thunderstorm is based on the monitoring of the electrical charge densities, the computation of the electric field and the production of lightning flashes. The cloud charging involves mostly the non-inductive mechanism, and both Intra-Cloud (IC) and Cloud-to-Ground (CG) flashes are considered.

As shown in [3], the model reproduced an extreme dry thunderstorm environment, responsible for a perfect scenario to natural ignition and fire propagation. The spatial distribution of Meso-NH-CELLS simulated CG lightning showed a good agreement with the lightning flashes obtained from the national lightning detection system.

## Acknowledgements

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# MODELLING ATMOSPHERIC CONDITIONS LEADING TO LARGE FIRES IN PORTUGAL

**Catia Campos<sup>1,2</sup>, Flavio T. Couto<sup>1,2</sup>, Rui Salgado<sup>1,2,3</sup>**

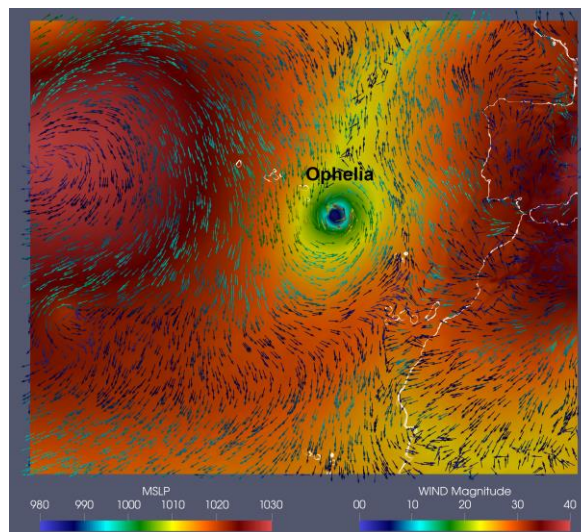
<sup>1</sup> Instituto de Ciências da Terra – ICT (Polo de Évora), Universidade de Évora, Évora, Portugal

Email : [m47661@alunos.uevora.pt](mailto:m47661@alunos.uevora.pt), [fcouto@uevora.pt](mailto:fcouto@uevora.pt), [rsal@uevora.pt](mailto:rsal@uevora.pt)

<sup>2</sup> Earth Remote Sensing Laboratory (EaRS Lab), Universidade de Évora, Évora, Portugal

<sup>3</sup> Departamento de Física, Escola de Ciências e Tecnologia, Universidade de Évora, Évora, Portugal

The extensive study of wildfires is crucial to better understand how fire may be influenced by the atmospheric conditions [1]. The study explores the meteorological conditions associated with the mega fires occurred in Portugal on 15 October 2017. For that purpose, the MesoNH [2] atmospheric model was used. The model can represent the atmospheric motions in different scales and was configured in different resolutions aiming to investigate the events in different temporal and spatial scales. For example, one of the simulations was configured in a large domain (300x250 grid points) and 15 km resolution aiming to represent the synoptic conditions. In this context, the simulation well represented the evolution of the hurricane Ophelia near Portugal [Figure 1], indicating the important role played by the weather system inducing strong south-westerly winds over Portugal in the late afternoon of 15 October. An experiment at higher resolution confirms the generation of intense gusts that favoured the rapid spread of the fires.



**Figure 1.** Mean sea level pressure (unit: hPa; coloured areas) and surface wind speed (unit: m/s) and direction (unit: m/s; arrows) at 0000 UTC on 15 October 2017.

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# Measurements of evaporation in Mediterranean and Antarctica lakes

**Miguel Potes<sup>1,2,3</sup>, Gonçalo Rodrigues<sup>1,2,3</sup>, Elena Shevnina<sup>5</sup>, Rui Salgado<sup>1,2,4</sup>, Maria João Costa<sup>1,2,4</sup>**

<sup>1</sup> Earth Remote Sensing Laboratory (EaRS Lab), Universidade de Évora, Rua Romão Ramalho, 59, 7000-671 Évora, Portugal

email: mpotes@uevora.pt

<sup>2</sup> Instituto de Ciências da Terra—ICT (Polo de Évora), Universidade de Évora, Rua Romão Ramalho, 59, 7000-671 Évora, Portugal

<sup>3</sup> Instituto de Investigação e Formação Avançada (IIFA), Universidade de Évora, Palácio do Vimioso, Largo Marquês de Marialva, 7002 - 554 Évora, Portugal

<sup>4</sup> Universidade de Évora, Departamento de Física, Escola de Ciências e Tecnologia, Rua Romão Ramalho 59, 7000-671 Évora, Portugal

<sup>5</sup> Finnish Meteorological Institute (FMI), Helsinki, Finland

The eddy covariance method is known worldwide as the accurate method to measure the evaporation in the natural ecosystems. Many artificial lakes were constructed in the Mediterranean region due to decrease in the annual precipitation. On the other hand, natural lakes are increasing in the Antarctica region due to loss of glacial melting resulting from the increase of ambient temperature caused by climate change. Continuous measurements with an IRGASON (Integrated CO<sub>2</sub> and H<sub>2</sub>O Open-Path Gas Analyzer and 3-D Sonic Anemometer) are being performed in Alqueva reservoir, Southeast of Portugal, since 2017. This set of measurements allows to calculate the evaporation of the reservoir through the eddy covariance method. In 2018, a similar instrument has been installed side-by-side for an intercomparison campaign of two weeks. Further in the austral summer, the second instrument has been installed in an Antarctica glacial lake during the ice-free period. The lake Zub/Priyadarshini is located in the Schirmacher oasis, Dronning Maud Land, East Antarctica. Evaporation results from these two different lakes, as well as from the intercomparison campaign are shown in this work. Evaporation during summer months in the Alqueva reservoir can reach 11 mm per day while in the lake Zub/Priyadarshini up to 5 mm per day. From the intercomparison campaign it results that the instrumental error of the second instrument (installed in the Antarctica lake) was 7%.

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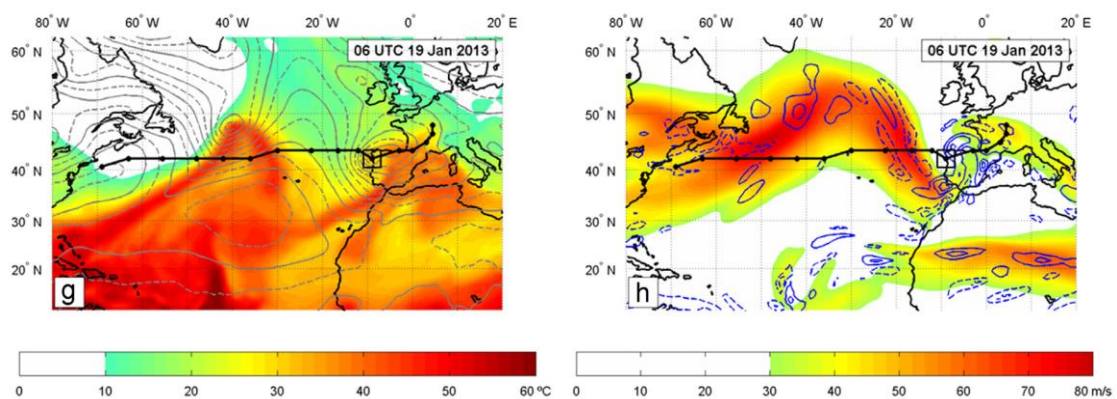
# DINAMIC AND DIABATIC PROCESSES IN EXTRATROPICAL CYCLONES IN THE ATLANTIC REGION

**Margarida L. R. Liberato**<sup>1,2</sup>

<sup>1</sup> Universidade de Trás-os-Montes e Alto Douro, UTAD, Quinta de Prados, 5000-801 Vila Real, Portugal  
email: mlr@utad.pt

<sup>2</sup> Instituto Dom Luiz (IDL), Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal

Extratropical cyclones (EC), also known as midlatitude cyclones, midlatitude storms, wind storms, frontal cyclones, have been studied for over 200 years. EC are one of the most prominent features of the midlatitude climate and represent a major mechanism for poleward transport of heat and moisture [1]. They are low pressure systems in the middle-latitudes and are frequently associated with heavy rain and strong winds. The occurrence of extreme windstorms is considered as one of the major natural catastrophes in the extratropics, being one of the costliest natural hazards in Europe, responsible for substantial socioeconomic damages and fatalities [2]. In this paper the conceptual models of EC are revisited, to understand the structure, evolution and underlying dynamics of the mid-latitude cyclone life cycle. Finally, the relative importance of baroclinic and diabatic processes for cyclone's intensification is discussed by means of recent extreme examples occurring in the Northeastern Atlantic region [3].



**Figure 1.** Large-scale conditions associated with the development of the cyclone Gong [2].

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# OBSERVED GEOMAGNETIC FIELD ANOMALIES AND POSSIBLE CONSEQUENCES

Maria Rosa Duque<sup>1</sup>

<sup>1</sup>Departamento de Física da Universidade de Évora, ECT. Rua Romão Ramalho nº 59, 7000-671 Évora.  
Email: [mrاد@uevora.pt](mailto:mrاد@uevora.pt)

Geomagnetic field data recorded by Magnetic Observatories, located in the Iberian Peninsula, at the end of February 1969, and inserted in Anais of the Observatories referred in the form of average hourly values of the vertical field, horizontal field and magnetic declination [1],[2] were used in the present work. The analysis of the records studied shows the occurrence of identical anomalies in days 26th and 27th but with less amplitude in day 26th. At the end of the great variation occurred on day 27 it is observed in all the Observatories an increase of the vertical component by about 9-10 nT and a decrease of the horizontal component from -35 to -22 nT. The comparison of the values obtained in Coimbra on February 26<sup>th</sup> and 27th shows an increase in the intensity of the field, between hour 10 and hour 15, which is essentially due to an increase in the horizontal component of the field. Another increase was observed, between hours 18 and 20, which is essentially due to an increase in the vertical component of the field. Given that these are variable magnetic fields, we can say that the horizontal component may be associated with ion movement in the vertical direction while the increase of the vertical component of the field may be associated with horizontal movement of ions. If this hypothesis is valid, we could have had, on the 27th, mainly vertical followed by mainly horizontal, ion movements. Between hours 14 and 17 there were large variations in the horizontal component and in the vertical component that led to significant changes in the slope and direction of the field. Thus, we will have electric fields associated with magnetic fields changing in intensity and direction, in an ocean environment.

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## Energia e Física Aplicada



# ANODE-LESS SECONDARY LITHIUM BATTERY: OPTIMIZATION OF THE DISCHARGE PLATEAU

**Manuela C. Baptista,<sup>1</sup> M. Helena Braga<sup>2</sup>**

<sup>1</sup> Engineering Physics Department, FEUP, University of Porto, 4200-465 Porto, Portugal

email: mbaptista@fe.up.pt

<sup>2</sup> LAETA-INEGI, Engineering Physics Department, FEUP, University of Porto, 4200-465 Porto, Portugal

email: mbraga@fe.up.pt

The national energy and climate plan for 2030 is the main energy and climate policy instrument. As such, all member states of the European commission work on their plan, considering greenhouse gas emissions, renewable energy, energy efficiency, energy security, internal market and research, innovation, and competitiveness as well as a straightforward approach to achieving the targets [1]. To accomplish these goals it is essential to develop energy harvesting and storage devices, namely for applications in vehicles, networks, industry, databases, wearables, and IoT [2].

In this work, we present batteries with an industrial efficient configuration, the assembly does not include a Li-metal anode [3]; the Li-metal plates upon the first charge.

At the same time, it is intended to combine the great advances achieved by the scientific community with the anode-less technology (mostly using liquid-state electrolyte) to the solid-state ferroelectric Li-rich electrolyte of the  $\text{Li}_3\text{ClO}$  family, in order to obtain a full solid-state anode-less battery.

This battery embraces several challenges including the optimization of the Cu sheet surface on the anode side. Charging should result in the deposition of a stable Li metal layer on the top of the current collector anode surface. In addition, optimizing the operating conditions during the charge/discharge steps, namely temperature and pressure is an additional endeavour. With all these strategies it is desired that the discharge plateau is as high as possible, in other words, that the internal resistance of the cell is reduced.

However, always keep in mind that with this new battery configuration it is possible to follow an economical path to high energy density, as well as safe and environmentally friendly battery.

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# CAPACITIVE EFFECT IN RECHARGEABLE SODIUM SEAWATER BATTERIES

**João Ferreira,<sup>1</sup> Tiago Salgueiro<sup>2</sup>, João Ventura<sup>3</sup>, Joana de Oliveira<sup>4</sup>**

<sup>1</sup>Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre 1021 1055, 4169-007 Porto, Portugal  
email: up201704185@edu.fc.up.pt

<sup>2</sup>Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre 1021 1055, 4169-007 Porto, Portugal

<sup>3</sup>Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre 1021 1055, 4169-007 Porto, Portugal

<sup>4</sup>Faculdade de Engenharia, Universidade do Porto, Rua Dr Roberto Frias, s/n 4200-465, Portugal

Humanity is reaching a tipping point where new sustainable energy solutions are needed. Rechargeable sodium seawater battery (SWB), assume the world leadership of high voltage batteries in marine environment [1-2]. With natural seawater as the active material, the SWB can be supplied infinitely with Na cations. Because of their open structure cathode, the performance of the battery is dependent on the characteristics of the cathode material, such as its surface area and hydrophilicity, being the goal to study their influence on the SWB performance. Three cathodes were studied in full SWB cell, two commercially available carbon felts (CF) with, approximately,  $2 \text{ m}^2\text{g}^{-1}$  of surface area, one pristine (PCF) and one heated (HCF), and an activated carbon felt (ACF) with a surface area of approximately  $2000 \text{ m}^2\text{g}^{-1}$ . The electrochemical performance of each cathode was evaluated with cyclic voltammetry and charge-discharge cycling tests, with currents ranging from 0.025 to 0.2 mA. The wettability of each cathode was also analyzed. The redox reactions involved in SWB are slow electrochemical processes [3]. With increased surface area, a much faster capacitive mechanism arises with an important contribution of the electric double layer capacitor (EDLC) formed at the cathode interface. In this work was possible to analyze the mutual influence of the capacitive and electrochemical energy storage mechanisms, with different carbonaceous cathodes. By applying a heat treatment, the CF hydrophilicity was increased facilitating the catholyte's access to the surface of the CF leading to an improvement of the battery performance, seen in the voltage profiles of PCF and HCF. The plateau attributed to the redox reactions and the slope due to the EDLC formation are compared. By improving the access to the surface, a small EDLC capacitive effect was observed, and simultaneously more active sites were available for the redox reactions. The improvement is also seen in the voltage gap, with the HCF presenting a smaller one than the PCF. The improvement becomes more significant when we compare the previous voltage profiles with the one with ACF. Here the initial slope is larger, not really reaching a plateau as stable as the ones with PCF and HCF within the 5 hours charge/discharge. This is due to the enormous increase in surface area of ACF which leads to a significant EDLC capacitive contribution. A lower voltage gap is also observed in this case with a faster charge due to an interface resistance decrease [3]. By comparing three CF with different characteristics, we were able to conclude that the cathode properties are an important factor in its performance. The surface area and SWB capacitive behavior were correlated and analyzed. A capacitive behavior leads to an increased power, which may be a key factor for some maritime energy storage applications, where a high surface cathode needs to be a priority.

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# ENERGY HARVESTING AND STORAGE TEXTILE-BASED DEVICE FOR SELF-POWERED WEARABLE ELECTRONICS

**R. S. Costa**,<sup>1,2</sup> **A. L. Pires**,<sup>1</sup> **A. M. Pereira**,<sup>1</sup> **C. Pereira**<sup>2</sup>

<sup>1</sup> IFIMUP, Department of Physics and Astronomy, Faculty of Sciences, University of Porto, Porto, Portugal  
email: rucosta@fc.up.pt

<sup>2</sup> REQUIMTE/LAQV, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Porto, Portugal

The paradigm of Sustainable Energy combined with the new Era of IoT boosted the search for self-powered devices that harvest and store energy, in order to satisfy the electrical needs of the generation of autonomous wearable electronics [1]. Thermally-chargeable supercapacitors are a clean energy technology that can convert the waste thermal energy into electrical energy (as a power source) and, simultaneously, store that energy (as an energy storage system). These hybrid devices allow converting the waste thermal energy provided from low-grade heat sources (*e.g.*, human body) into electrical energy through the thermally-induced migration of electrolyte ions towards the electrodes based on the Soret effect [1,2].

In this work, we report on the fabrication of a thermally-chargeable textile supercapacitor (T-TSC) composed of two multiwalled carbon nanotube-coated cotton electrodes (MWCNT@cotton) and an all-solid-state ionic polyelectrolyte. The MWCNT@cotton electrodes were prepared by directly coating the cotton substrates with a MWCNTs dispersion through a scalable dip-pad-dry process. The T-TSC was fabricated by sandwiching the ionic polyelectrolyte between the MWCNTs/cotton electrodes. The thermally-induced power generation of the T-TSC was evaluated, reaching an output potential of up to 30 mV for an applied temperature gradient of 25 K. The thermal charging process occurred in two stages, leading to a Soret coefficient value of 1.85 mV/K obtained by linear fitting of the  $\Delta V/\Delta T$  curves in the range of  $\Delta T = 11\text{--}25$  K. Concerning the energy storage results, the T-TSC presented an electric double-layer charge storage mechanism, affording a working potential of 2.27 V and an energy density of 4.33 Wh/kg at a power density of 620 W/kg. The high flexibility and the efficient performance of the T-TSC, combined with the scalable and cost-effective fabrication process, make this device a feasible solution to satisfy the challenges of self-powered wearable electronics.

## Acknowledgements

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# IMPROVING HEMATITE PERFORMANCE FOR GREEN HYDROGEN PRODUCTION BY SOLAR WATER SPLITTING

**João Pedro Freitas<sup>1</sup>, Paula Quitério<sup>1</sup>, Rita Simões<sup>1</sup>, Célia T. Sousa<sup>1,2</sup>, Sérgio Magalhães<sup>3</sup>, Tânia Lopes<sup>4</sup>, Adélio Mendes<sup>4</sup>, João P. Araújo<sup>1</sup> and Arlete Apolinário<sup>1</sup>**

<sup>1</sup> The Institute of Physics for Advanced Materials, Nanotechnology and Photonics (IFIMUP), Laboratory of Physics for Materials and Emergent Technologies (LaPMET), Department of Physics and Astronomy, Faculty of Sciences – University of Porto, Rua do Campo Alegre s/n, 4169-007, Porto, Portugal  
email: [joao.freitas@fc.up.pt](mailto:joao.freitas@fc.up.pt)

<sup>2</sup> Departamento de Física Aplicada, Facultad de Ciencias – Universidad Autónoma de Madrid, Ciudad Universitaria de Cantoblanco, C. Francisco Tomás y Valiente, 7, 28049, Madrid, Spain

<sup>3</sup> Technological and Nuclear Campus (CTN), Instituto Superior Técnico – University of Lisbon, Estrada Nacional 10, km 139, 7, 2695-066, Bobadela, Lisbon, Portugal

<sup>4</sup> Laboratory for Process Engineering, Environment, Biotechnology and Energy (LEPABE), Department of Chemical Engineering, Faculty of Engineering – University of Porto, Rua Sr. Roberto Frias, 4200-465, Porto, Portugal

Hydrogen (H<sub>2</sub>) as a source of energy has been gaining popularity in recent years, yet about 96 % of the H<sub>2</sub> currently produced still derives from fossil fuels. Photoelectrochemical (PEC) cells arise as a clean and less spending alternative for the production of green H<sub>2</sub> through solar water splitting [1]. Hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) is considered a promising semiconductor for PEC cells due to its narrow optical band gap (2.2 eV), long-term stability and natural abundance, reaching 16.8 % solar-to-hydrogen efficiency in theory. This work focuses on the development and optimization of efficient photoanodes based on hematite, combined with different improvement strategies: nanostructuring, elemental doping and surface modifications. Photoanodes based on 1D bare hematite nanowires (NWs) were obtained through hydrothermal method [2]. Then, an elemental doping approach for hematite NWs was performed, testing Sn, Mn, Co and Ti as doping elements. Mn and Ti were the most promising dopants, hence an optimization on the doping concentration in terms of the materials photoresponse was performed. Improvements of 37 % and 15 % on the photocurrent density (*j*) were obtained for 7 % Mn and 1 % Ti doping, respectively, when compared with bare hematite. Regarding the onset potential (*V*<sub>OC</sub>), a 70 mV shift was achieved for 1 % Mn doping from bare hematite. Rutherford Backscattering Spectrometry associated with X-Ray Diffraction allowed the study of the dopant distribution through the hematite crystalline structure. Furthermore, Scanning Electron Microscopy enabled the morphology analysis and UV-Vis spectroscopy the determination of optical band gaps.

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# MAGNETIC TUNNEL JUNCTIONS EMBEDDED WITH PARAMAGNETIC CENTERS FOR ENERGY HARVESTING

**Maria Grácio<sup>1</sup>, Elvira Paz<sup>2</sup>, Ricardo Ferreira<sup>2</sup> and Joao Ventura<sup>1</sup>**

<sup>1</sup> Faculty of Sciences of the University of Porto, Rua do Campo Alegre, s/n, 4169-007, Porto, Portugal  
email: up201705000@fc.up.pt

<sup>2</sup> International Iberian Nanotechnology Laboratory, Avda. Mestre José Veiga s/n, Braga, Portugal

A huge development in magnetic nanostructures has been witnessed in the latest decades, due to the growing interest in Spintronics, a research area that uses the spin of electrons as an additional degree of freedom. Unlike conventional electronics, spintronic devices take advantage of the spin of electrons to obtain, transmit and process information, with increased efficiency. Magnetic tunnel junctions (MTJs) [1] are the most successful implementation of this technology. These devices consist of a series of stacked nanometric layers, with the critical effects occurring at the interfaces between the magnetic layers and the insulator. By the application of an external magnetic field, the magnetic layers can be parallel or anti-parallel aligned, offering two different resistance states. This device is used in data storage and processing, namely in hard disk read heads, and in the prominent MRAM.

Here, we present a study on the physical properties of these devices, namely the appearance of an electromotive force (emf) in MTJs with paramagnetic impurities in the tunnel barrier [2]. For this, we fabricated MTJ samples with MgO tunnel barriers (which presents an important spin filtering mechanism that enhances TMR ratios) doped with Ta impurities. We performed the electrical characterization by measuring current-voltage (I-V) curves and magnetoresistive hysteretic cycles and measured the dependence their temperature dependence (300 – 20 K). We obtained TMR ratios of approximately 70%, from junctions with resistance area products of approximately 4 M $\Omega\mu\text{m}^2$ . Our I-V results will be explained in terms of tunneling across the barrier and the effect of Ta impurities-doping within the tunneling barrier.

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# Increase the Performance of the Thermoelectric Generator Thought Printed Collectors

A. L. Pires<sup>1</sup>, M.M. Maia<sup>1</sup>, M M. Rocha<sup>1</sup>, P. Robalinho<sup>2</sup>, J. Silva<sup>3</sup>, O. Frazão<sup>2</sup>, A. M. Pereira<sup>1</sup>

<sup>1</sup>IFIMUP - Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Faculdade de Ciências da Universidade do Porto, 4169-007 Porto, Portugal.

<sup>2</sup>INESC - Institute for Systems and Computer Engineering, Technology and Science, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal.

<sup>3</sup>CeNTI - Centre for Nanotechnology and Smart Materials, Famalicão, Portugal

e-mail: [ana.pires@fc.up.pt](mailto:ana.pires@fc.up.pt)

One of the strategies to boost the temperature difference in the thermoelectric generators (TEGs) can be through the use of collectors or/and plasmonic systems [1]. In the present work, the influence of several screen-printed collectors will be used to study their impact on the final performance of the TEGs. For that, several TEGs were produced by screen-printing and using p-type Bi-Te-based inks, as reported in [2], in a radial configuration. In this thermoelectric configuration, the heat will be made from the center of the device by using a laser with a wavelength of 1500 nm. Additionally, titanium nitrate (TiN), Zinc Oxide, and bismuth oxide (Bi<sub>2</sub>O<sub>3</sub>)-based nanomaterials inks or even commercial carbon-based materials were screen printed in the center of the TEG. The printed collectors with a thickness between 80 to 100 μm were analyzed by UV-Vis-NIR reaching an absorbance higher than 90%. With the present work, we will demonstrate that implementing a collector increased the generated temperature gradient by 50%, leading to an overall performance increase of ~ 47%.

Finally, as proof of concept, the produced collectors were accomplished to a thermoelectric generator. A complete characterization of the outputs was performed before and after the application of each collector.

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# ENERGY HARVESTING COMBINING THERMOMAGNETIC MATERIALS AND TRIBOELECTRIC NANOGENERATORS

**R. Bugalhão<sup>1\*</sup>, C. Rodrigues<sup>1</sup> and J. Ventura<sup>1</sup>**

<sup>1</sup>IFIMUP and Department of Physics and Astronomy, University of Porto, Portugal  
email: up201606052@up.pt

Energy is increasingly one of the major and most important forces on our society, making its generation and harvesting a broadened studied topic. Due to this high demand for the distribution of electrical power, the interest in Energy Harvesting (EH), the concept of converting unused ambient energy from our surrounding environment into electrical energy, is increasing. Amongst the various available external sources, thermal energy is one of the most researched for the purpose of EH, not only because it is the most ubiquitous one, but also for being the form of energy that all the others are eventually turned into. Thermal EH relies on "free heat", so a beneficial alternative of a green energy source would be to capture this lost heat, convert it into electrical energy and use it to re-power devices.

Thus, our study focuses on researching a device that performs such conversion in the low-grade temperature range. Our setup is composed of a NdFeB permanent magnet on top of a hot source and a triboelectric nanogenerator (TENG) directly above a cold source. Between them is a thermomagnetic material (TMM) with a Curie Temperature ( $T_c$ ) near 23 °C (e.g. Gd) where an oscillatory motion is forced through heating and cooling. When heated above  $T_c$ , Gd transitions from ferromagnetic to paramagnetic and falls on the TENG, generating an energy peak. Then, the Gd is cooled below  $T_c$ , leading to a paramagnetic-ferromagnetic phase transition. When that occurs, the Gd is once again attracted by the permanent magnet and lifts off the TENG, generating another energy peak. This cycle repeats as long as the TMM's temperature oscillates around  $T_c$ .

Here, we present a study on how physical properties of TMMs such as  $T_c$  or thickness influence the energy generation, optimum resistance or oscillation frequency of the proposed device, aiming for its optimization and potential assessment. Although these values depend on several parameters, the best results obtained so far were an open circuit voltage of 8 V, a short circuit current of 0,36  $\mu$ A and a motion frequency of 66 mHz, for a TMM with  $T_c = 39,9$  °C and a zigzag PTFE-Nylon TENG.

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# MAGNETOSTRICTIVE SENSORS FOR STRUCTURAL MONITORING OF CORROSION IN CRITICAL ASSETS

**J. Silva,<sup>1</sup> B. Moreira,<sup>2</sup> M. Sadeghi,<sup>1</sup> A. M. Pereira,<sup>1</sup> G. Dinis,<sup>2</sup> C. Gouveia<sup>2</sup>**

<sup>1</sup> IFIMUP - Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, rua do Campo Alegre s/n, 4169–007 Porto, Portugal

<sup>2</sup> EQS Global, Rua Joaquim Dias Rocha, n.º 354 Zona Industrial da Maia 1, sector X, 4470-211 Maia, Portuga  
email:

In 2019, 614 pipeline incidents were reported in the US alone. It is estimated that between 50% and 60% of these incidents are caused by corrosion, aging and wear of the pipeline material[1]. Such defects go unnoticed until a leakage or a spillage occur. The inspection of these assets is often hard and expensive, so new methods are necessary.

Non-destructive testing is used to determine the integrity of infrastructure without compromising its operation. Pipelines are structures that particularly benefit from these tools, since they are generally long, opaque, and hard to reach.

The MAGSENSE project aims at developing a solution to the inspection of such assets. By combining a magnetostrictive transducer with ultrasound signal processing, a new system emerges. The layout of the system consists of a magnetostrictive material which provides the transduction between magnetization and vibration, thus generating sound waves. The transducer is magnetized by a permanent and a perpendicular alternating magnetic field. The frequency of the magnetic field defines the frequency of the acoustic wave. Changes in the magnetization are detected by a pick-up coil adjacent to the transducer. The sounds waves are emitted and received by the same sensor-actuator. Any defects that are encountered by the sound wave as it travels the pipe are reflected. Further signal processing allows to determine the distance at which those defects are located.

Different configurations of the sensor-actuator allow different analyses to be performed on the pipe, namely along its length (crack, holes, etc.) and the thickness (wall thinning, corrosion, etc.).

The MAGSENSE project is a collaboration between three groups, EQS Global, IFIMUP (UP) and CMEMS (UM). The goal of the project is to develop the inspection system entirely and to apply it in a real industrial environment.

## Acknowledgements

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# CORRENTES GEOMAGNETICAMENTE INDUZIDAS AGREGAM INDÚSTRIA E CIÊNCIA

**Rute Rodrigues Santos<sup>1,2</sup>, Maria Alexandra Pais<sup>1</sup>, Joana Alves Ribeiro<sup>1,3</sup>,  
Fernando Pinheiro<sup>1</sup>, João Cardoso<sup>2</sup>**

<sup>1</sup>Univ. Coimbra, CITEUC, Department of Physics, Coimbra, Portugal

<sup>2</sup>Univ. Coimbra, LIBPhys, Department of Physics, Coimbra, Portugal

<sup>3</sup>Univ. Lisboa, Instituto Dom Luiz, Lisboa, Portugal

O Sol emite continuamente partículas e radiação eletromagnética em todas as direções. Estas emissões energéticas podem atingir a Terra onde, por interação com a magnetosfera e a ionosfera, originam tempestades geomagnéticas que induzem campos elétricos na Terra condutora. Ao longo de infraestruturas condutoras aterradas, como as linhas de transmissão de energia, os campos elétricos induzidos fazem circular as correntes elétricas conhecidas por GICs (Correntes Geomagneticamente Induzidas).

No âmbito do Projeto MAG-GIC: *Correntes geomagneticamente induzidas em Portugal continental*, modelizámos e medimos o efeito das GICs na rede nacional de transporte de energia [1], operada pela REN (Redes Eléctricas Nacionais). Por motivo deste projeto, desde 2018 que existe uma parceria entre indústria e ciência, tendo por elemento aglutinador as GICs. Essa parceria trouxe à ciência os valores dos parâmetros que permitiram simulações realistas. Quanto à indústria, beneficiou da colaboração através do cálculo de estimativas de GICs, que permitiram avaliar o nível de risco na sua rede de transporte. De realçar ainda outra componente importante do projeto – a multidisciplinaridade da equipa científica. A colaboração com diferentes áreas científicas (Geofísica, Física Aplicada, Geologia, Meteorologia Espacial), tornaram este projeto mais abrangente e consistente.

Tendo por pano de fundo o tema das GICs, que será devidamente introduzido, esta comunicação pretende também partilhar a experiência do relacionamento dos últimos 4 anos entre uma equipa de investigadores e uma equipa da REN. Ao longo de reuniões regulares, discussão de relatórios, escrita de artigos, os olhos que olharam para as GICs não viram exatamente a mesma coisa...

## Acknowledgements

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## Posters

# AQUISIÇÃO E TRATAMENTO DE DADOS EXPERIMENTAIS COM A CALCULADORA GRÁFICA

**J. Jorge Teixeira<sup>1</sup>, Ana M. Dias<sup>2</sup>**

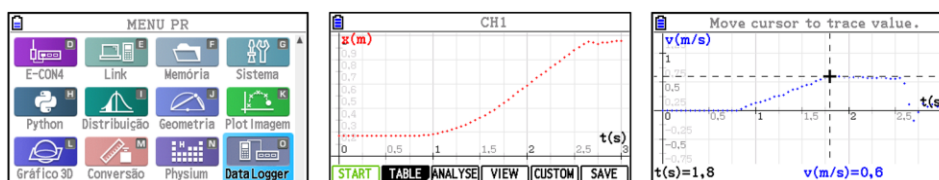
<sup>1</sup> Agrupamento de Escolas Dr. Júlio Martins, Av. 5 de outubro, 5400-017 Chaves, Portugal.

email: jjsteixeira@gmail.com

<sup>2</sup> Casio School Coordinator, Rua do Polo Sul, n.º 2 4.ªA, 1990-273 Lisboa, Portugal.

Cada vez mais alunos e professores de Física e Química A recorrem à calculadora gráfica (CG) em atividades que requerem o traçado de gráficos e de retas de ajuste aos dados experimentais. Os exames nacionais de Física e Química A incluem questões cuja resolução requer o recurso a uma CG. Assim, a CG é uma tecnologia que o aluno, no ensino secundário, tem de ter disponível e a única a que pode aceder nos exames. Para a aquisição e tratamento de dados experimentais, professores e alunos utilizam, normalmente, diverso *software* e *hardware*, sendo necessário algum tempo de familiarização. Quanto maior for o número de programas e instrumentos utilizados, menos tempo os alunos têm disponível para outras tarefas como, por exemplo, previsão de resultados, tratamento de dados, comunicação de resultados, discussão de resultados, etc. Deste modo, somos de opinião que a utilização da CG pelos alunos, em conjunto com uma aplicação específica, é uma mais-valia no processo ensino/aprendizagem ao nível da rentabilização do tempo, dos custos e da utilização de metodologias ativas. Para o efeito, foi criada, em 2021, a aplicação *Data Logger* para as calculadoras CASIO [1].

Assim, este trabalho tem como principais objetivos mostrar as potencialidades da aplicação *Data Logger*, indicar alguns exemplos de atividades (figura 1) e apresentar um manual para o professor com sugestões, montagem do material, procedimento para a recolha de dados com a calculadora e o tratamento de dados recolhidos nas atividades laboratoriais de Física dos 10.º e 11.º anos. A realização das atividades laboratoriais com a aplicação referida foi implementada numa turma do 10.º ano, constituída por 18 alunos. Verificou-se que a utilização simultânea da CG e da aplicação *Data Logger* foi um fator de motivação para os alunos, o número de ensaios realizados pelos alunos duplicou, todos os alunos partilharam os resultados com a turma e houve uma melhoria de 19% nas questões dos testes relacionadas com as atividades laboratoriais, em relação às atividades laboratoriais de química onde não utilizaram a CG.



**Figura 1.** Alguns ecrãs da calculadora obtidos numa atividade experimental.

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# Un fascinante recurso didáctico: la cámara termográfica

## Prada, F.<sup>1</sup>, Cassinello, P.<sup>2</sup>

<sup>1</sup>Dpto. Física y química. I.E.S. Las Lagunas. Rivas-Vaciamadrid (Madrid). España. (Miembro de la DEDF).  
email: [fernando.pradaperez@educa.madrid.org](mailto:fernando.pradaperez@educa.madrid.org)

<sup>2</sup> Dpto. Física y química. IES Diego Velázquez (Madrid). España. (Miembro de la DEDF).  
email: [pablo.cassinello@educa.madrid.org](mailto:pablo.cassinello@educa.madrid.org)

“Una imagen vale más que mil palabras”, este proverbio sintetiza perfectamente la idea de que las imágenes proporcionadas por las cámaras termográficas son más claras y provechosas que la mera explicación verbal de un proceso termodinámico. Las imágenes termicas captan la atención del estudiante y le sorprenden, invitándole a explorar y aprender. (Figura 1)

### Objetivos

- Mejorar la comprensión de la física, hacerla más atractiva e impulsar vocaciones científicas.
- Ofrecer un innovador recurso didáctico que facilita el trabajo del docente.

### Metodología

La facilidad de manejo de las cámaras termográficas hace posible su aplicación en diferentes actividades didácticas: explicaciones en el aula, experiencias de laboratorio, investigaciones de campo, aplicaciones técnicas de iniciación profesional o demostraciones en ferias de ciencia.

- Entre los numerosos procesos susceptibles de ser visualizados y analizados directamente bajo la mirada infrarroja, se encuentran [1]: efecto invernadero, efecto Joule, cambios de estado, formas de transferencia de calor, disipación de energía, compresión adiabática, etc. (Figura 2)
- Y entre las investigaciones de campo y aplicaciones técnicas [2]: detección de fugas térmicas en edificios, detección de humedades y filtraciones de agua, análisis de eficiencia energética, comparativa de materiales aislantes y detección de recalentamientos en cuadros eléctricos.



**Figura 1.** La visión termográfica actúa como un catalizador del aprendizaje de la física.

**Figura 2.** Visualización del efecto botijo; demostración realizada en el stand de la RSEF (gestionado por la DEDF) durante la Feria Madrid por la Ciencia y la Innovación (2019).

### Conclusiones

Las cámaras térmicas, además de visibilizar fenómenos térmicos invisibles a simple vista, ofrecen una tecnología que impulsa la motivación del estudiante y contribuye a la mejora de la calidad de enseñanza. Por todo ello, no deberían faltar en ningún centro educativo.

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# POLARIZACIÓN CIRCULAR CON GAFAS PARA PELÍCULAS 3D

Cassinello, P.<sup>1</sup>, Prada, F.<sup>2</sup>

<sup>1</sup> Dpto. Física y Química IES Diego Velázquez. Torrelodones. Madrid. España (Miembro de la DEDF) [pablo.cassinello@educa.madrid.org](mailto:pablo.cassinello@educa.madrid.org)

<sup>2</sup> Dpto. Física y Química IES Las Lagunas. Rivas-VaciaMadrid (Madrid). España (Miembro de la DEDF) [fernando.pradaperez@educa.madrid.org](mailto:fernando.pradaperez@educa.madrid.org)

En bastantes ocasiones sólo se estudian los polarizadores lineales. Proponemos experiencias para abordar también con los estudiantes, los de tipo circular realizadas simplemente con un material asequible y barato: las gafas polarizadas para ver películas en tres dimensiones.

## Objetivos

- Mejorar la comprensión y atracción de la Física e impulsar vocaciones científicas
- Comprobar aplicaciones sorprendentes de los polarizadores circulares que suscitan el interés en aprender sobre qué es la polarización, sus tipos y qué es birrefringencia.

## Metodología

Una primera experiencia se basa en la birrefringencia. Si se colocan celos delante de una pantalla (que emite luz polarizada) y a continuación se coloca otro polarizador se obtienen vivos colores por la birrefringencia del cielo. Para una misma disposición de celos, puede explicarse que los colores son diferentes dependiendo de interponer un polarizador lineal cruzado, lineal paralelo o circular. Los del paisaje de la Fig.1 se han conseguido con un polarizador circular. La birrefringencia además de espectacular, es importante pues es el fundamento de la visualización de imágenes y vídeos de todos los dispositivos que utilizan pantallas de cristal líquido[1]

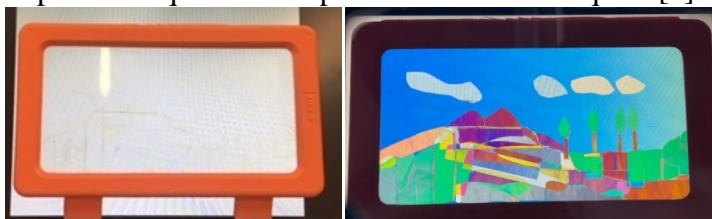


Fig.1. Izq. Celos sin polarizador. Dcha. Mismos celos, al interponer el polarizador circular de una gafa 3D

Otra de las experiencias con polarizadores circulares que explicaremos consiste en el oscurecimiento selectivo de una moneda (Fig. 2). Se dispone un polarizador circular encima de una moneda y un letrero que pueden verse con detalle. Pero, si damos la vuelta al plástico, sólo la moneda se vuelve totalmente oscura.



Fig.2. Izq. Moneda y letrero vistos con el plástico de gafa 3D. Der. Mismos objetos al dar la vuelta al plástico.

## Conclusiones

Puede conseguirse aplicaciones sugerentes de la polarización circular mediante los plásticos polarizadores de una gafa de 3D. Contribuyen a aumentar la motivación del estudiante y la mejora en la calidad de la enseñanza de la Óptica.

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# ANODIC WO<sub>3</sub> SELF-ORDERED NANOPORES FOR SOLAR WATER SPLITTING AND GREEN HYDROGEN GENERATION

**Rita Simões,<sup>1\*</sup> Paula Quitério<sup>1</sup>, João Pedro Freitas<sup>1</sup>, Célia T. Sousa<sup>1,2</sup>, Vanessa Lima<sup>3</sup>, Adélio Mendes<sup>4</sup>, João P. Araújo<sup>1</sup> and Arlete Apolinário<sup>1</sup>**

<sup>1</sup>The Institute of Physics for Advanced Materials, Nanotechnology and Photonics (IFIMUP), Laboratory of Physics for Materials and Emergent Technologies (LaPMET), Dep. Fís. e Astron, Faculty of Sciences - University of Porto (FCUP), Rua do Campo Alegre s/n, 4169-007, Porto, Portugal;

<sup>2</sup>Departamento de Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid (UAM), Campus de Cantoblanco, C/ Francisco Tomás y Valiente, 7, M 12 604 - 28049, Madrid, Spain;

<sup>3</sup>Centro de Tecnologias Estrategicas do Nordeste (CETENE), Av. Prof. Luís Freire, 1 - Cidade Universitária, Recife - PE, 50740-545, Brazil;

<sup>4</sup>Laboratory for Process Engineering, Environment, Biotechnology and Energy (LEPABE), Dep. Eng. Química, Faculty of Engineering - University of Porto (FEUP), s/n, R. Dr. Roberto Frias, 4200-465 Porto, Portugal

\*email: up201703960@edu.fc.up.pt

Much attention has been brought to nanostructured tungsten trioxide (WO<sub>3</sub>) for its potential applications as a stable photoanode for solar water splitting and as photocatalyst for hydrogen production. Many morphologies of nanostructured WO<sub>3</sub>, like nanopores (NPs), nanotubes (NTs), nanoplates, nanorods, among others, can be synthesized by several fabrication techniques including hydrothermal, solgel, electrodeposition, and anodization [1,2]. In this work, we explored the fabrication of anodic nanostructured WO<sub>3</sub> layers by the W foil electrochemical anodization, which few reports have addressed so far. A detailed investigation was conducted on the influence of the anodization conditions [electrolyte type and concentration, applied anodization voltage and synthesis duration time] in the formation of self-ordered nanopores/NTs. These parameters impact and effect on the growth of stable and organized anodic WO<sub>3</sub> NPs was obtained by SEM morphology characterization and the growth mechanism and rate of the nanoporous WO<sub>3</sub> layers were monitored and analyzed by the current density and charge anodization curves. Furthermore, for the first time reported, Co and Ni doped WO<sub>3</sub> layers were obtained by pulsed anodization. The effects of Cobalt(II) sulfate heptahydrate concentration in the electrolyte and anodization/deposition pulse durations on the oxide morphology and photo-performance were studied. Structural characterization of the resulting doped layers was performed using Raman Scattering and X-Ray Diffraction. Optimized samples with a higher degree of NPs organization, oxide thickness and doping elements were characterized in terms of their photoresponse performance (by photocurrent-voltage curves) to evaluate their solar-to-hydrogen efficiency and by UV-Vis spectroscopy to determine the optical band gaps.

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# **PROBLEMS ASSOCIATED WITH THE CONTRAST BETWEEN THERMAL AND MECHANICAL PROPERTIES OF MATERIALS**

**Maria Rosa Duque<sup>1</sup>**

<sup>1</sup>Departamento de Física da Universidade de Évora, ECT. Rua Romão Ramalho nº 59, 7000-671 Évora.  
Email: [mrاد@uevora.pt](mailto:mrاد@uevora.pt)

The present work consists in the study of thermal and mechanical properties of a body consisting of the same volume of two materials with different thermal and mechanical properties,[1],[2] placed in physical contact. The materials are subjected to a common thermal source but, due to their density and specific thermal capacity, their temperatures will suffer different variations. This work studies the changes occurring near the contact zone of the two materials. In addition to different volume increases (pressure increases) in the two materials, different values of thermal conductivity must be considered and shear stresses of thermal origin, presenting different values in the two materials must be studied near the contact zone. The work consists of the study of the changes observed near the contact area of the two materials considering different values of heat supplied. Changes of thermal conductivity values with temperature are considered but variations with pressure increase are not considered.

The hypothesis of introducing a third element (water) into pre-existing cracks dilated with the initial heating is also studied. Special attention is given to the content of this third element as well as to the effect of the temperature increase in the body and the contact border between the two initial materials.

This work was carried as part of research work at the University of Evora, Portugal

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# Superconductivity in antiperovskites

Noah Hoffmann<sup>2</sup>, **Tiago F.T. Cerqueira**<sup>1</sup>, Jonathan Schmidt<sup>2</sup>, and Miguel A. L. Marques<sup>2</sup>

<sup>1</sup>CFisUC – Centro de Física da Universidade de Coimbra, Departamento de Física, Universidade de Coimbra, Rua Larga, 3004-516 Coimbra, Portugal

<sup>2</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany  
email: tiagoc@uc.pt

Perovskites are a family of compounds with unique electrical properties that make them promising candidates for use in a variety of electronic devices. One field where perovskites have a pivotal role is superconductivity. In fact, the cuprate ceramics that hold the record for the highest transition temperature ( $T_c$ ) belong to this family. In this work, we present a comprehensive theoretical study of conventional superconductivity in cubic antiperovskites materials with composition  $XYZ_3$  where X and Z are metals, and Y is H, B, C, N, O, and P. Our starting point are electron-phonon calculations for 397 materials performed with density-functional perturbation theory. We discovered 16 compounds close to thermodynamic stability and with  $T_c$  higher than 5K, including antiperovskites with Y=H, N, C and O. We then used these results to train interpretable machine learning models to understand and further explore this family of compounds. This leads us to predict a further 57 (thermodynamically unstable) materials with superconducting transition temperatures above 5K.

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# PYCOIMBRA: AN OPEN-SOURCE CODE FOR WILDFIRE PROPAGATION STUDY

**Daniel Neves<sup>1\*</sup>, João Aveiro<sup>1</sup>, A.M.G. Lopes<sup>2,3</sup>, C. Viegas<sup>2,3</sup>, Jaime Oliveira da Silva<sup>1</sup>**

<sup>1</sup>CFisUC, Department of Physics, University of Coimbra, 3004-516 Coimbra, Portugal

<sup>2</sup>Univ Coimbra, Departamento de Engenharia Mecânica, Rua Luís Reis Santos, Pólo II, 3030-788 Coimbra

<sup>3</sup>ADAI (Associação para o Desenvolvimento da Aerodinâmica Industrial)

\* email: nevesdanielf@gmail.com

Over the past few decades, wildfires have become a significant concern in our society [1].

In this work, we present an open-source python-based software of fire simulation using the semi-empirical Rothermel's fire spread model [2] coupled with an ellipse-type model (single or double) to describe fire shape [3] and a wind field simulator [4].

The simulation incorporates different types of fuel and can deal with any terrain and wind direction configuration, to match practically any real-world scenario.

For each cell on a two-dimensional rectangular lattice, we consider 16 neighbouring cells for application of a Dijkstra type algorithm, to sort out ignition times, rate of spread and compute the fire path. By doing so, we are able to define a graph structure that could be the base for fire suppression studies.

The python programming language is chosen due to its readability and modular capability for rapid new developments and advances in fire simulation

## Acknowledgements

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# Phase diagrams of high-pressure ternary systems

**João N.Q. Oliveira<sup>1</sup>, Fernando Nogueira<sup>1</sup>, and Tiago F.T. Cerqueira<sup>1</sup>**

<sup>1</sup>CFisUC – Centro de Física da Universidade de Coimbra, Departamento de Física, Universidade de Coimbra, Rua Larga, 3004-516 Coimbra, Portugal

email: jmnqoliveira@gmail.com

High pressure has led researchers into finding higher and higher critical temperature superconductors, continuously breaking the record for the highest  $T_c$  material. For example, room-temperature superconductivity was claimed in a photochemically synthesised ternary carbonaceous sulfur hydride system (H-C-S) at 15 °C and 267 GPa [1]. However, given the high pressure apparatus used, researchers are often unable to determine the crystal structure of these superconductor compounds. This is one of the many examples where theory and computation play well with experiment: because theorists are not limited by apparatus, they can help in discovering the structure of these new compounds. This can be done using specialised methods to search for the lowest energy structure of a given composition, an approach called crystal structure prediction (CSP). In this work, we applied CSP methods to predict the lowest energy structures of compounds in the H-C-Se, H-Mg-Se and Li-C-S ternaries. In total, we analysed 37 different compositions at 150 GPa. We then studied their thermodynamics and electronic structure in order to estimate which of them may have a higher chance of being superconductors.

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# Computational Structure Prediction of Low-Dimension Systems

**Pedro Borlido<sup>1,3</sup>, Miguel Marques<sup>2</sup>, Silvana Botti<sup>3</sup>**

<sup>1</sup>CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal  
email: pedro.borlido@uc.pt

<sup>2</sup> Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

<sup>3</sup> Institut für Festkörperteorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

With the increase of computational power, ab-initio electronic structure methods have not only become a valuable companion in the characterization of materials but also a reliable tool for their prediction. Coupled with efficient global optimization methods, we can now explore entire composition ranges using only a (powerful enough) computer, discover the most interesting and most likely to be stable, and use this information to maximize the chance to synthesize new materials. Thanks to their versatility, these global optimization methods are efficiently adapted for problems of different dimensionality: 3D (bulk material discovery[1]), 2D (two-dimensional systems, grain boundaries[2]), 1D (grain boundaries in 2D systems) and 0D (point defects in solids[3]).

In this work, we present a small general discussion on global optimization methods, focusing on the Minima Hopping Method[4], and use this context to discuss some results on quasi-two-dimensional systems of particular technological interest for the silicon industry: 2D-Si[5] and 2D-SiH[6]. Although honeycomb silicene is the prototypical system when we think of 2D-Si, it is far from being the most stable. In fact, derivative atomic arrangements (e.g. dumbbell formation) can lead to much stabler structures which are in addition semiconducting. The addition of adsorbates such as hydrogen explodes the number of possible arrangements but also critically changes the type of the observed structures. These results offer some insight in the structuring of low-dimension silicon which could prove useful in attempting their synthesis and experimental study.

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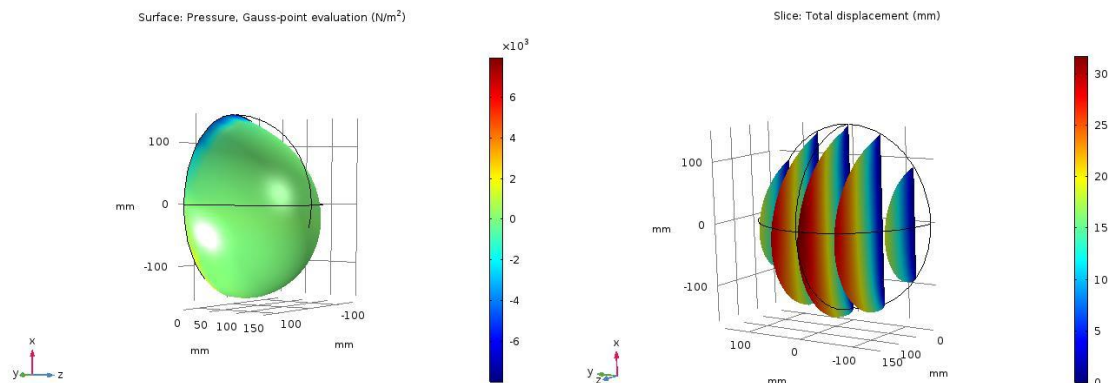
# Modelação 3D de fantasmas da mama

Tesesa Borges<sup>1</sup>, M. Duarte Naia<sup>1,2</sup>

<sup>1</sup>ECT/UTAD - School of Science and Technology, University of Trás-os-Montes e Alto Douro, Vila Real, Portugal. email: silvanacabo\_guedes@hotmail.com; duarte@utad.pt

<sup>2</sup>CEMMPRE, Centre for Mechanical Engineering, Materials and Processes, Coimbra, Portugal

A imagiologia da mama melhorou a deteção precoce do cancro da mama, com impacto na taxa de mortalidade e na qualidade de vida em sobrevivida. No entanto o diagnóstico errado afeta todos os anos muitas mulheres [1]. Aumentar a sensibilidade e especificidade das imagens médicas continua a ser objeto de investigação e desenvolvimento, a maior dificuldade na investigação detalhada em imagiologia do corpo humano deve-se ao custo e ao risco para o paciente [2]. Consequentemente os fantasmas, digitais e físicos, constituem uma ferramenta essencial para o desenvolvimento de novas técnicas e dispositivos. Com eles podem simular-se uma quantidade quase ilimitada de anomalias anatómicas e melhorar o conhecimento e avaliação quantitativa, comparação e melhoria das tecnologias com imagens médicas com métodos fiáveis a baixo custo [3]. O propósito desta trabalho é fundamentalmente o desenvolvimento de fantasmas digitais para a simulação de imagens radiológicas com modelos de estruturas e propriedades de estados normais patológicos. Os modelos foram implantados e estudados com a plataforma de simulação numérica COMSOL Multiphysics [4],



**Figura 1-** Pressão superficial e deslocamento da mama sujeita uma força de contacto vertical e ação da gravidade.

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# GRAPH THEORY APPROACH TO WILDFIRE SUPPRESSION

**João Aveiro<sup>1\*</sup>, Daniel Neves<sup>1</sup>, Paulo Silva<sup>1</sup>, Orlando Oliveira<sup>1</sup>, Fernando Nogueira<sup>1</sup>,  
Jaime Oliveira da Silva<sup>1</sup>**

<sup>1</sup>CFisUC, Department of Physics, University of Coimbra, 3004-516 Coimbra, Portugal

\* email: jpd.aveiro@gmail.com

Several algorithmic approaches based on graph theory are used to optimize the suppression of wildfire propagation. The nodes of the graph that models the propagation represent a raster cell of a terrain grid and each edge corresponds to the time required for a burning cell to propagate to the adjacent cells, as provided by the Rothermel equations [1]. An effective propagation is obtained by considering a set of ignition cells and computing the multi-source shortest path via the Dijkstra's algorithm.

Suppression efforts are modelled by the removal, either permanent or temporary, of a graph node that, in this way, constrains the set of terrain cells that are combustible. An effective suppression is achieved via the minimization of the number of burnt cells at a target time  $t_{final}$ , whilst also minimizing the removal, i.e. the suppression, of grid cells, decreasing the suppression effort. This effectively constitutes a network interdiction problem [2] of NP-hardness.

Several approaches based on classical graph algorithms are presented together with a heuristic one based on the use of genetic algorithms. A comparison of the performance of these methods, including some remarks regarding the computational cost, is discussed.

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# Ab-initio studies of $\text{Bi}_2\text{Se}_3$ , $\text{Bi}_2\text{Te}_3$ , and $\text{Bi}_2\text{Se}_{3-x}\text{Te}_x$

**Ana Fontes<sup>1</sup>, Fernando Nogueira<sup>1</sup>, and Pedro Borlido<sup>1</sup>**

<sup>1</sup> CFisUC – Centro de Física da Universidade de Coimbra, Departamento de Física, Universidade de Coimbra, Rua Larga, 3004-516 Coimbra, Portugal  
email: anabpfontes@gmail.com

Topological insulators are materials with an energy gap in the bulk but with topologically protected conducting surface states. These materials have garnered a lot of attention due to their potential usefulness in, e.g., spintronics. The bismuth chalcogenides are an extensively studied family of topological insulators, with  $\text{Bi}_2\text{Se}_3$  as a prototypical material, given its relatively simple surface states and its almost ideal Dirac cone [1].  $\text{Bi}_2\text{Se}_3$  is often doped with Te to compensate for Se vacancies. Different doping patterns lead to different transport properties. In this work, we present a computational study of the substitutional alloys  $\text{Bi}_2\text{Se}_{3-x}\text{Te}_x$  using cluster expansion methods. Calculations were done using a plane-wave expansion of the Kohn-Sham equations of Density Functional Theory [2], using the Local Density Approximation exchange and correlation functional, with the D2 van der Waals corrections of Grimme et al. [3]. Starting from ab-initio calculations of small inequivalent supercell configurations, we estimate the density of states, the lattice parameters, and the energy gap as a function of the concentration of Te.

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# Large scale screening of high refractive index materials

**Pedro J.M.A. Carrico<sup>1</sup>, Pedro Borlido<sup>1</sup>, Márcio Ferreira<sup>1</sup>, and Tiago F.T. Cerqueira<sup>1</sup>**

<sup>1</sup> CFisUC – Centro de Física da Universidade de Coimbra, Departamento de Física, Universidade de Coimbra, Rua Larga, 3004-516 Coimbra, Portugal  
email: pj.carrico@gmail.com

Modern optics industry requires transparent materials with large refractive indices ( $n$ ), as they are key ingredients in the design of wave-guides, optical interference filters, mirrors and anti-reflection coatings. Commercially, only a handful of materials are relevant, since the band gap is inversely proportional to the refractive index. The computational search for new high- $n$  materials is hindered by the fact that (although not the most excruciating property to compute) the refractive index is still considerably more expensive to calculate than, for example, a formation energy. Even considering the constant effort of the community to bypass this deficiency, the largest scale datasets of this quantity contain approximately 5000 entries, piling in comparison to the plethora of known materials [1, 2].

Machine learning has become a prominent subject in materials science due to the promise of high accuracy at a much lower computational cost than standard methods. Among the recent state of the art methods in use are crystal graph convolution networks (CGNNs) [3]. CGNNs are neural networks that operate on graph-structured data. The network consists of a series of connected nodes, each of which represents a vertex in the graph. The edges of the graph are used to connect the nodes and define the relationship between them.

In this work, we trained a CGCNN to predict the refractive index of a recently published dataset of 175k stable and metastable materials [4]. For the most promising candidates, we performed Density Functional Theory calculations to validate the results. A good agreement between predictions and calculations was observed, and a few interesting candidates with high refractive index were identified.

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# First-principles calculation of superconducting transition temperature of Al-Li-Pd ternary materials

**Josué Vermelo<sup>1</sup>, Fernando Nogueira<sup>1</sup>, and Tiago F.T. Cerqueira<sup>1</sup>**

<sup>1</sup> CFisUC – Centro de Física da Universidade de Coimbra, Departamento de Física, Universidade de Coimbra, Rua Larga, 3004-516 Coimbra, Portugal  
email: javermelo1@gmail.com

Although high- $T_c$  superconductors have drawn the attention of the public away from conventional superconductors, the discovery of  $MgB_2$  superconducting behaviour spawned a new interest on the latter [1]. Superconducting transition temperatures may not be high enough to allow access to the superconducting state with nitrogen cooling, but the ductility of these materials is a clear advantage in the fabrication of wires over the brittle ceramics typical of high- $T_c$  compounds. From a theoretical point of view, conventional superconductors offer yet another advantage: the mechanism behind the superconducting state is known. The ab-initio determination of electronic structure, phonons and electron-phonon couplings using Density Functional Theory is well-established and has proven to be accurate enough for the determination of superconducting transition temperatures using the Allen–Dynes-modified McMillan equation [2]. In this work, we applied this method to the Al-Li-Pd family of ternary materials. Firstly, we applied crystal structure prediction methods to predict the ground state structure of 19 compositions within this family, and found 18 close to the thermodynamic stability. From these, 13 were previously unreported in the literature [3]. We then proceeded to calculate the superconducting critical temperature of the metallic phases.

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# COMBINED LOCAL PROBE AND AB-INITIO STUDY OF DION-JACOBSON LAYERED STRUCTURES

**Pedro A. Sousa<sup>1</sup>, António N. Cesário<sup>1</sup>, E. Lora da Silva<sup>1</sup>, P. N. Lekshmi<sup>1</sup>, P. Rocha Rodrigues<sup>1</sup>, J. G. Correia<sup>2</sup>, J. P. Araújo<sup>1</sup> and A. M. L. Lopes<sup>1</sup>**

<sup>1</sup>IFIMUP, Faculdade de Ciências da Universidade do Porto, Portugal,

email: up201704307@edu.fc.up.pt

<sup>2</sup>C2TN, Centro de Ciências e Tecnologias Nucleares, Departamento de Engenharia e Ciências Nucleares, Instituto Superior Técnico, Portugal

## INTRODUCTION

Hybrid improper ferroelectricity was found in some A'AB<sub>2</sub>O<sub>7</sub> Dion-Jacobson oxides, which like Ca<sub>3</sub>Mn<sub>2</sub>O<sub>7</sub>, are also naturally layered perovskites, consisting also of a stack of perovskite layers, two octahedra thick, but intercalated with a distinct arrangement set of large A'-cations (A' = Cs or Rb). By substituting the A' cation ions in systems as in A'NdB<sub>2</sub>O<sub>7</sub>, (B = Nb, Ta), several structural factors can be tuned modifying consequently the relative overlapping of adjacent perovskite blocks, and also the degree of octahedra tilting and rotation within the perovskite layers. [1]

## EXPERIMENTAL STUDY

Dion Jacobson compounds CsNdB<sub>2</sub>O<sub>7</sub> (B = Nb, Ta) were synthesized following the solid-state technique. For A = K we need to perform an ion-exchange following the path: Rb → Na → K. The phase purity and crystal structure analysis were carried out using X-ray powder diffraction (Rigaku SmartLab X-Ray Diffractometer). The PAC experiments with temperature dependence were made using a 6-BaF<sub>2</sub> detector spectrometer [2] equipped with a dedicated closed-cycle refrigerator or with a special high-temperature furnace.

## THEORETICAL STUDY

Using the Quantum Espresso (QE) code, we performed first-principles electronic-structure calculations for CsNdB<sub>2</sub>O<sub>7</sub> (B = Nb, Ta). With the presence of the 4f-orbital of Neodymium (Nd), the system behaves as a metal. Thus, we need to use the Hubbard model to treat our system correctly, since it will make half-filled orbitals less energetically favorable.

## RESULTS AND DISCUSSION

We report the evolution of structural proprieties for CsNdB<sub>2</sub>O<sub>7</sub> (B = Nb, Ta) with the support of PAC results, which leads to a better understating of the phase transitions and phase stabilities of CsNdB<sub>2</sub>O<sub>7</sub>.

With DFT calculations, we determined the Hubbard parameter that best describes these DJ phases and confirm that the system behaves as an insulator, with the study of the Partial Density of States (PDOS) of the two systems.

## CONCLUSION

With our results, we are closer to the understanding of this promising and fascinating materials from the Dion-Jacobson family, which presents a huge number of applications and are crucial to the revolution of the technological world.

## Acknowledgements

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# FLEXIBLE TOPOLOGICAL INSULATORS THIN FILMS FOR MAGNETO-ELECTRIC SPIN ORBIT

Mário Gustavo Barbosa Santos, Sofia Ferreira Teixeira, Ana Lúcia Mota Pires,

André Miguel Trindade Pereira

<sup>1</sup>IFIMUP, Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Department of Physics and Astronomy, Faculty of Sciences, University of Porto, Portugal  
Email: up201606269@edu.fc.up.pt

In 1965 Gordon Moore stated that the number of transistors in an integrated circuit had been doubling every two years and predicted that it would be so for at least the next ten years<sup>[1]</sup>. That prediction remained true throughout the subsequent years, earning the name of Moore's law. However, as sizes reach the order of the nanometre, it becomes clear that Moore's law is faltering, and soon alternatives must arise so technological progress can proceed. That is where spintronics comes in, relaying on spin-charge coupling to produce more efficient data storage devices. The work here presented focused on applying spin orbit torque to magnetic material. We centred our research on Topological Insulators (TIs), materials that present a large spin-orbit coupling that allows a high spin to charge conversion through the devices based on spin Hall effect.

To achieve that purpose, we produced thin films using magnetron sputtering deposition of TIs, namely  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$ , over glass and Kapton substrates. Deposition conditions were manipulated to achieve the best crystalline structure possible, changing parameters such as current intensity (in a range of 20mA to 80mA) and the temperature of the substrate in situ (in a range of 100°C to 350°C). Additionally, we resorted to post-thermal annealing with an Argon flux to improve the films' structure. The morphology of the film was viewed by SEM images and evaluated using XRD measurements. XRR measurements were also conducted to determine the thickness of the films, obtaining results between 6.8 and 16.1 nm.

The films' resistances and Seebeck coefficients were measured at room temperature and at varying temperatures (range from approximately 15K to 300K)<sup>[2]</sup>. For  $\text{Sb}_2\text{Te}_3$  films conductivity decreased for lower deposition temperatures (results varied from 70S/m to 2573S/m) and higher current intensities (from 63S/m to 25S/m). As for the Seebeck coefficient, a slight increase was verified for higher deposition intensities (from 233  $\mu\text{V/K}$  to 373  $\mu\text{V/K}$ ), and the inverse was true for higher deposition temperatures (from 125 $\mu\text{V/K}$  to 229 $\mu\text{V/K}$ ). The  $\text{Bi}_2\text{Te}_3$  films presented slight change in the Seebeck coefficient for different deposition current intensities (between 42  $\mu\text{V/K}$  and 64  $\mu\text{V/K}$ ), however the conductivity spanned from 14000S/m to 29000S/m.

All these results will be fully discussed in the present work.

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# SIMULAÇÃO MECÂNICA DE UM STENT

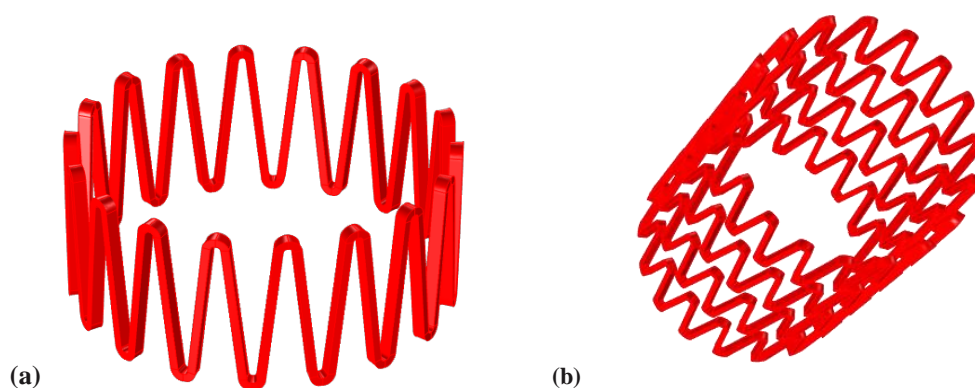
**Filipa B. Araújo<sup>1</sup>, M. Duarte Naia<sup>1,2</sup>**

<sup>1</sup>ECT/UTAD – School of Science and Technology, University of Trás-os-Montes e Alto Douro, Vila Real, Portugal.

email: filipabaraujo@sapo.pt; duarte@utad.pt.

<sup>2</sup> CEMMPRE, Centre for Mechanical Engineering, Materials and Processes, Coimbra, Portugal.

Os stents são dispositivos com estrutura tubular que colocados no interior de um ducto permitem mantê-lo aberto. A implementação desta tecnologia no sistema vascular revolucionou a cirurgia vascular, em particular a angioplastia cardiovascular. O stent ideal deve apresentar biocompatibilidade e excelente resistência à corrosão. A estrutura forma uma malha que permite evitar a oclusão ou estenose do lúmen que pode ser induzida por diversas patologias. Os problemas que advêm destas doenças, assim como do desenvolvimento destes dispositivos, podem ser simulados e estudados através de modelos numéricos, em particular, utilizando métodos de elemento finitos. Neste trabalho mostra-se os resultados de simulação um modelo de um stent criado com as características e o material adequado, ou seja, com as condições mecânicas necessárias para ser possível observar o comportamento mecânico nas condições de funcionamento. O modelo também foi aplicado na simulação do escoamento do sangue num vaso e na interação do stent com a parede e o sangue para avaliar a sua degradação. A figura 1 mostra o modelo: em 1(a) observa-se o anel, suficiente para avaliar o comportamento mecânico e em 1(b) mostra-se o modelo do stent completo, que permite analisar o escoamento e a evolução da interação com o meio.



**Figura 1.** Representação do modelo do stent criado na aplicação na Comsol Multiphysics: (a) Anel do modelo do stent – para avaliação do comportamento;(b) Modelo do stent para simulação do escoamento.

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# ARCHITECTURED MATERIALS FOR ELECTROMAGNETIC SHIELDING TEXTILES

Ana Rita Sousa<sup>1,2</sup>, José Barbosa<sup>3</sup>, O. Salomé G.P. Soares<sup>3</sup>, João Ferreira<sup>4</sup>, Ana L. Gonçalves<sup>4</sup>, Gilda Santos<sup>4</sup>, Augusta Silva<sup>4</sup>, José Morgado<sup>4</sup>, Patrícia Soares<sup>5</sup>, Sergey A. Bunyaev<sup>1</sup>, Gleb N. Kakazei<sup>1</sup>, Cristina Freire<sup>2</sup>, M. Fernando R. Pereira<sup>3</sup>, Clara Pereira<sup>2</sup>, André M. Pereira<sup>1</sup>

<sup>1</sup>IFIMUP - Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Physics and Astronomy Department, Faculty of Sciences, University of Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal.

<sup>2</sup>REQUIMTE/LAQV, Chemistry and Biochemistry Department, Faculty of Sciences, University of Porto, Rua do Campo Alegre s/n, 4169-007, Porto, Portugal.

<sup>3</sup>LSRE-LCM, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.

<sup>4</sup>CITEVE - Technological Centre for the Textile and Clothing Industry of Portugal, Rua Fernando Mesquita, 2785, 4760-034 Vila Nova de Famalicão, Portugal.

<sup>5</sup>Cottonanswer, Rua dos Combatentes do Ultramar, 50, 4750-047 Lijó, Barcelos, Portugal

The progress of humanity is accompanied by the boost of data transfer and communication technologies. The recent 5G technology implementation is drastically different from older technologies since the electromagnetic (EM) radiation frequency will be several orders higher, going up to the millimetric wave band. This has led to an increase in the levels of EM radiation in the environment, that may affect human health and the performance of electronic devices due to the EM interference [1]. Such issue is instigating the scientific community to search and develop innovative materials for EM shielding that can replace typical metallic-based shields and, preferentially, block EM radiation by absorption rather than by reflection. Carbon materials, conductive polymers, metal oxides and their nanocomposites are examples of such materials [2].

In this work, different types of materials belonging to the abovementioned groups were used to develop electromagnetic shielding textiles for a wide range of applications and their performance was assessed and compared. The materials were incorporated onto textile substrates by different techniques (*e.g.*, coating, screen-printing, dip-coating). The EM shielding effectiveness (SE), given in decibel (dB), was measured between 5.85 and 18 GHz by the transmission line test.

Several promising formulations were achieved that produced uniform textiles with efficient electromagnetic shielding properties. SE values >30 dB and >60 dB were obtained using different combinations of conductive polymers, carbon materials and magnetic nanoparticles, which are classified as excellent for general use and professional use textile applications, respectively [3]. Effective EM shielding textiles that are flexible, lightweight and cost-effective were produced that display competitive SE for electronic industries and protective garments.

## Acknowledgements

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# NOVEL APPLICATIONS OF TRIBOELECTRIC ENERGY HARVESTING IN REMOTE AND HARSH ENVIRONMENTS

**C. Rodrigues, A. Pereira, J. Ventura**

IFIMUP and Faculty of Sciences of the University of Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal.  
email: catia.rodrigues@fc.up.pt

To reliably obtain data in remote and harsh environments is one of the most difficult achievements of the information age we live in. Although the Internet of Things revolution is connecting billions of sensors that provide an unsurmountable amount of data, there is one thing all these devices still need: electrical power [1,2]. Therefore, we will here demonstrate energy harvesting strategies able to power low consumption sensors in two of the harshest and less monitored environments on Earth: oil extraction wells and the ocean.

The monitoring of oil & gas extraction wells is an increasing need to prevent major disasters. However, present solutions to feed sensors are inefficient, costly and risky. As a solution, triboelectric nanogenerators (TENGs) [1] are a new powerful mean to generate electrical power from random mechanical motions based on the coupling of the contact electrification with electrostatic induction effects [1,2]. In this work it was demonstrated a TENG able to generate electrical energy in harsh conditions similar to those found in extraction wells (pressures up to 830 bar and temperatures up to 120 °C) in direct contact with methane and crude oil [3]. The electrical performance of the assembled device shows that temperature is the most critical parameter for TENGs operating in harsh environments.

Providing energy to offshore floating equipment is a challenging task, given their typical remote location at sea. Wave energy is a highly dense and abundant resource that can be exploited and as a solution to harvest this blue energy, three different rolling-sphere-based TENGs were developed. Their performance compared in both a “dry” bench testing system under rotating motions, and in a large-scale wave basin under realistic sea-states installed within a scaled navigation buoy [4]. Experiments shows that the voltage generated by the TENGs increases with increasing wave frequency and amplitude, achieving maximum values for periods close to the natural period of the buoy (~ 0.920 s). The wave basin tests clearly demonstrated the need to take into account the full dynamics of the buoy, and not only that of TENGs, when subjected to the excitations of waves.

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# NANO-FEATURES EFFECT ON TRIBOELECTRIC NANOGENERATORS OUTPUT PERFORMANCE

**Ana C. P. da Silva<sup>1</sup>, Cátia R. S. Rodrigues<sup>2</sup>, Maria Pilar Pina<sup>3</sup>, Reyes Mallada  
Viana<sup>3</sup>, João O. Ventura<sup>2</sup>, André M. Pereira<sup>2</sup>**

<sup>1</sup>IFIMUP - Institute of Physics for Advanced Materials, Nanotechnology and Photonics  
email: carolinasilva@fc.up.pt

<sup>2</sup>IFIMUP - Institute of Physics for Advanced Materials, Nanotechnology and Photonics

<sup>3</sup>INMA – Institute of Nanosciences and Materials of Aragon

## Abstract

The upcoming Internet of Things era, in which several sensorized devices gather and exchange data in real time, brought the need to develop integrated energy harvesting technologies. In particular, since these small electronics require a reduced amount of power, nanogenerators provide an effective solution for this issue.

The triboelectric nanogenerator (TENG) is a technology that has the advantage of converting low-frequency mechanical energy into electricity, allowing the powering of small devices such as self-powered sensors or wearable electronics. Due to their simple assembling, stability and cost-efficiency, they are considered a promising sustainable power source.

Since its discovery, the development of strategies to enhance the TENG output performance has been one of the main research topics in this field. Considering that this technology depends on the surface charge density on the material's surface, its improvement leads to an increase of the dipole moment between electrodes and, consequently, to a higher power output. Such an effect can be achieved using metamaterials – materials that are engineered in order to have custom properties not found in the original form.

Hence, in this work we discuss the effect of changing the materials properties by incorporating dielectric magnetic nanoparticles into PDMS at different concentrations. Moreover, the influence of gold clusters deposited on PMMA nano-structured surfaces is also studied.

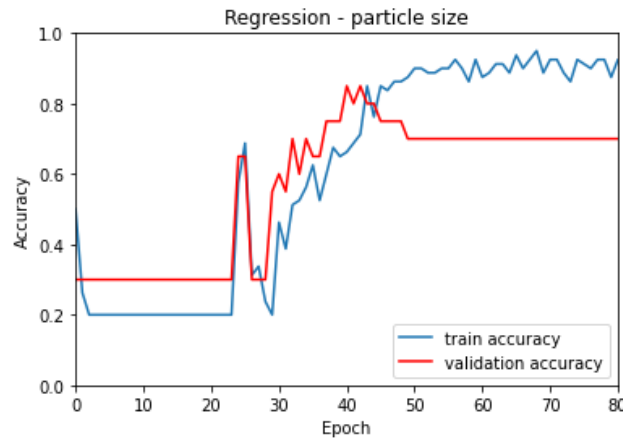
# NEURAL NETWORKS FOR OPTIMAL PARTICLE PARAMETERS

**José Miguel Pereira<sup>1\*</sup>, Daniel Santos<sup>1</sup>, Catarina Dias<sup>1</sup>, João Ventura<sup>1</sup>**

<sup>1</sup>IFIMUP, Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Portugal

\*up201805391@edu.fc.up.pt

Advances in improved construction materials benefit from the study of the reflective properties of nanoparticles doped coatings. Although finite-difference time-domain (FDTD) [1] simulations can be scaled to any frequency and size, the simulation of small structures such as nanoparticles in layers of a significantly bigger dimensions requires high resolution and therefore high computational power. This work was performed with the objective of reducing the number of simulations needed for a neural network that, with a certain color as input, could give the nanoparticles parameters able to maximize the reflectance. A neural network based on single particle simulations was created, significantly reducing the simulation time, with a compromise between other effects, and its output was used to extrapolate information for the multiple particles scenario. Simulations for various particles geometries and sizes (50 nm - 1  $\mu$ m) were performed using an open-source software package MEEP [2]. From them two distinct networks were created, a fully connected neural network (FCNN) that had color as an input and a convolutional neural network (CNN) that used the reflectance spectrum, both outputting a geometry from a classification and dimensions from a regression. The latter network showed a better accuracy (Figure 1).



**Figure 1.** Accuracy of the regression problem (particle size) in the CNN train.

## Acknowledgements

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# COMBINED LOCAL PROBE AND RAMAN STUDY OF RUDDLESDEN-POPPER LAYERED PEROVSKITES

**António Cesário**<sup>1</sup> **Pedro A. Sousa**<sup>1</sup> **E. Lora da Silva**<sup>1</sup> **P. N. Lekshmi**<sup>1</sup> **P. Rocha Rodrigues**<sup>1</sup> **J. G. Correia**<sup>2</sup> **J. P. Araújo**<sup>1</sup> and **A. M. L. Lopes**<sup>1</sup>

<sup>1</sup>IFIMUP, Faculdade de Ciências da Universidade do Porto, Portugal

email: antonio.cesario@fc.up.pt

<sup>2</sup>C2TN, Centro de Ciências e Tecnologias Nucleares, Departamento de Engenharia e Ciências Nucleares, Instituto Superior Técnico, Portugal

Hybrid Improper Ferroelectric (HIF) compounds constitute a promising set of materials, with recent studies aiming to fine tune their structures and develop materials with enhanced properties, such as polar (ferroelectric) phases. They offer a wide range of applications as magnetoelectrics or ferroelectric random access memories (FRAMs).

Polar symmetry with macroscopic polarization can be produced in ( $n = 2$ ) Ruddlesden-Popper (RP) layered compounds, with disconnected octahedra along [001], by introducing octahedra rotation or tilts, known as hybrid improper ferroelectricity (HIF). Two prototypical examples are the  $\text{Ca}_3\text{Mn}_2\text{O}_7$  (CMO) and  $\text{Ca}_3\text{Ti}_2\text{O}_7$  (CTO) compounds, where the former system has been proposed to present a unique coupling between its magnetic and ferroelectric orderings [1,2]. However, at room temperature, the CMO system is known to present, besides the polar  $A21am$  structural symmetry, a second non-polar structural phase. To increase the thermal stability of the ferroelectric symmetry, we studied a RP –  $\text{Ca}_3\text{Mn}_{2-x}\text{Ti}_x\text{O}_7$  doped system (CMTO).

This includes experimental work with Perturbed Angular Correlation (PAC), a technique where nuclear probes are exchanged with lattice sites, providing very sensitive information about the Hyperfine Interactions at those sites. Raman measurements were also taken with temperature to further study those transitions.

A structural phase, with the characteristics of the polar symmetry  $A21am$  previously reported in CMO was found in our CMTO compound at room temperature, possibly granting Hybrid Improper Ferroelectricity at such temperatures. However, at the time of writing, we have to further investigate the purity of this phase across the temperature range.

## Acknowledgements

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# EFFECT OF PARTICLE SHAPE IN GIANT MAGNETO-INDUCED DEFORMATION IN MAGNETOACTIVE ELASTOMERS

**J. A. Silva,<sup>1</sup> C. Gouveia<sup>2</sup>, G. Dinis<sup>2</sup>, A. M. Pereira<sup>1</sup>**

<sup>1</sup> IFIMUP - Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, rua do Campo Alegre s/n, 4169–007 Porto, Portugal  
email: asilva.joana@gmail.com

<sup>2</sup> EQS Global, Rua Joaquim Dias Rocha, n.º 354 Zona Industrial da Maia 1, sector X, 4470-211 Maia, Portugal

Magnetoactive elastomers (MAEs) are composites whose physical properties can be tuned with an external magnetic field. They are composed of a ferromagnetic filling embedded in a polymeric matrix. These materials have become attractive due to their capacity of changing stiffness and shape, thus finding application in controllable valves and vibration attenuators.

In this work we report the use of helix shaped FeCo soft ferromagnetic particles in silicone rubber. We have shown that the size and the particular shape of the particles enable giant magneto-induced strain (magnetostriction), even with volumetric concentrations below 5vol.%. Moreover, we report the effects of induced anisotropy on the magnetic, mechanical and magnetostrictive properties of the MAEs. Isotropic MAEs have shown to be invariant in tensile tests with and without magnetic field of  $H = 200$  Oe. On the other hand, anisotropic MAEs have shown to become softer with the application of an external field, and stiffer with increasing volume fraction. This is explained by the magnetostriction contribution to the strain of the material, given the anisotropic samples' higher sensitivity at low fields.

The physical mechanisms behind the magneto-induced changes in the physical properties are explained, based on the particle's morphological description. With this work we have shown that by tailoring the geometry of the magnetic filling in MAEs it is possible to achieve giant deformation rates using significantly lower particle concentrations.

## Acknowledgements

This work was financed by FEDER funds through the COMPETE 2020 - Operacional Programme for Competitiveness and Internationalisation (POCI), Portugal 2020, and by national funds (PIDDAC) through FCT/MCTES through the projects POCI-01-0247-FEDER-033783, NORTE-01-0145-FEDER-022096, UID/NAN/50024/2019. Joana Silva acknowledges the support of FCT through the grant SFRH/BD/143943/2019.

# Python code for solving simple quantum systems with the Numerov numerical method

Francisco Caruso<sup>1</sup>, Vitor Oguri<sup>2</sup>, Felipe Silveira<sup>2</sup>

<sup>1</sup> Centro Brasileiro de Pesquisas Físicas, Rua Dr. Xavier Sigaud, 150, 22290-180, Urca, Rio de Janeiro, RJ, Brazil

<sup>2</sup> Universidade do Estado do Rio de Janeiro, Rua São Francisco Xavier, 524, 205550-900, Maracanã, Rio de Janeiro, Brazil

email: felipe.silveira@uerj.br

A Python based code of the Numerov method [1,2] is developed in a didactic way with the use of *Jupyter Notebook* version 6.0.3 for three simple quantum systems: hydrogen atom; molecule governed by the Morse potential; and quantum dot [3]. The code, which is conceived to find the eigenfunctions and eigenvalues for those systems, will be made available in full, so that it can be used and improved.

## Acknowledgements

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# CORRENTES GEOMAGNETICAMENTE INDUZIDAS AGREGAM INDÚSTRIA E CIÊNCIA

**Rute Rodrigues Santos<sup>1,2</sup>, Maria Alexandra Pais<sup>1</sup>, Joana Alves Ribeiro<sup>1,3</sup>,  
Fernando Pinheiro<sup>1</sup>, João Cardoso<sup>2</sup>**

<sup>1</sup>Univ. Coimbra, CITEUC, Department of Physics, Coimbra, Portugal

<sup>2</sup>Univ. Coimbra, LIBPhys, Department of Physics, Coimbra, Portugal

<sup>3</sup>Univ. Lisboa, Instituto Dom Luiz, Lisboa, Portugal

O Sol emite continuamente partículas e radiação eletromagnética em todas as direções. Estas emissões energéticas podem atingir a Terra onde, por interação com a magnetosfera e a ionosfera, originam tempestades geomagnéticas que induzem campos elétricos na Terra condutora. Ao longo de infraestruturas condutoras aterradas, como as linhas de transmissão de energia, os campos elétricos induzidos fazem circular as correntes elétricas conhecidas por GICs (Correntes Geomagneticamente Induzidas).

No âmbito do Projeto MAG-GIC: *Correntes geomagneticamente induzidas em Portugal continental*, modelizámos e medimos o efeito das GICs na rede nacional de transporte de energia [1], operada pela REN (Redes Eléctricas Nacionais). Por motivo deste projeto, desde 2018 que existe uma parceria entre indústria e ciência, tendo por elemento aglutinador as GICs. Essa parceria trouxe à ciência os valores dos parâmetros que permitiram simulações realistas. Quanto à indústria, beneficiou da colaboração através do cálculo de estimativas de GICs, que permitiram avaliar o nível de risco na sua rede de transporte. De realçar ainda outra componente importante do projeto – a multidisciplinaridade da equipa científica. A colaboração com diferentes áreas científicas (Geofísica, Física Aplicada, Geologia, Meteorologia Espacial), tornaram este projeto mais abrangente e consistente.

Tendo por pano de fundo o tema das GICs, que será devidamente introduzido, esta comunicação pretende também partilhar a experiência do relacionamento dos últimos 4 anos entre uma equipa de investigadores e uma equipa da REN. Ao longo de reuniões regulares, discussão de relatórios, escrita de artigos, os olhos que olharam para as GICs não viram exatamente a mesma coisa...

## Acknowledgements

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# PRODUCTION OF Bi<sub>2</sub>Te<sub>3</sub> NANOPlates FOR THERMOELECTRIC NANOGENERATORS WITH HIGH PERFORMANCE

**Mariana Rocha**,<sup>1</sup> Margarida Maia<sup>1</sup>, Ana L. Pires<sup>1</sup>, André Pereira<sup>1</sup>

<sup>1</sup>IFIMUP – Instituto de Física de Materiais Avançados, Nanotecnologia e Fotónica, Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal  
email: mariana.rocha@fc.up.pt

During the past few decades, with rapid enlargement of human society, consumption of traditional energy has increased exponentially. Thermoelectric materials (TE) can generate electrical energy when they are exposed to a thermal gradient, considered almost the unique solutions for sustainable energy harvesting for recovering the wasted heat [1,2]. These materials present lightweight, small size, pollution free and recycling potential [2]. One of the most used TEs is the alloy Bi<sub>2</sub>Te<sub>3</sub> since it is considered as the best performing thermoelectrical material near room temperature (150–300 K).[2] The performance of a thermoelectric material is assessed by a dimensionless figure-of-merit,  $zT$ , defined as  $zT = S^2\sigma T/(\kappa_e + \kappa_l)$ , where  $S$ ,  $\sigma$ ,  $\kappa_e$ ,  $\kappa_l$  and  $T$  are the Seebeck coefficient, electrical conductivity, electronic and lattice thermal conductivities, and the absolute temperature, respectively. An average  $zT$  between 1.5–2 can enable substantial waste-heat harvesting and application in primary power generation [3]. Recently, in order to obtain high  $zT$  values, was developed Bi<sub>2</sub>Te<sub>3</sub> nanomaterials leading thus a strong quantum confinement and a significant reduction of the  $\kappa_e$  since the mean free path of phonons are much higher than of the electrons. This will cause an increase of the  $zT$  value [4].

In this work were prepared Bi<sub>2</sub>Te<sub>3</sub> nanoplates (NPs) using a modified chemical reduction process using, for the first time, an alkanolamine to decrease the NPs size and thickness as well as to increase the quantum confinement [5]. The NPs were characterized by XRD, TEM, SEM/EDS, and transport properties presenting a Bi<sub>2</sub>Te<sub>3</sub> phase,  $S = -62.0 - -113.6 \mu\text{V K}^{-1}$  (being n-type semiconductor),  $\sigma = 208 - 1203 \text{ S m}^{-1}$ , and a Power Factor of  $1.78 - 6.14 \mu\text{W m}^{-1} \text{ K}^{-2}$ .

## Acknowledgements

This work was funded by H2020-EU.1.2.1. - FET Open Project (WiPTherm, grant agreement ID: 863307).

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# HIGH CONCENTRATION MAGNETORHEOLOGICAL ELASTOMERS

**S. Maryam Sadeghi<sup>1</sup>, Joana Silva<sup>1</sup>, Carlos A. J. Gouveia<sup>2</sup>, Bruno Moreira<sup>2</sup>, Gabriel Dinis<sup>2</sup> and André M. Pereira<sup>1</sup>**

<sup>1</sup>IFIMUP, Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Department of Physics and Astronomy, Faculty of Sciences, University of Porto, Porto, Portugal

<sup>2</sup>EQS Global, 4470-211 Maia, Portugal

email: s.maryam.sadeghee@gmail.com

Magnetorheological elastomers (MREs) are elastic materials categorized as smart materials that have physical or mechanical properties significantly affected when under an external magnetic field [1]. MREs consist of ferromagnetic/superparamagnetic particles, an elastomer. With these 2 components could tailor the magnetic properties such as high saturation magnetization, high magnetic permeability, and low remanent magnetization [2]. In this work, isotropic and anisotropic MREs were fabricated through mixing Hiperco 50 particles in polydimethylsiloxane (PDMS) containing 9.2 to 25.6 vol.% of metallic powder. For isotropic samples, magnetostriction measurements were performed and high values up to 5560 ppm were obtained with 9.2 vol.% of Hiperco particles under a field of  $H=6500$  Oe. Then, it decreased slightly when a higher metal content was employed (5300, 4680, 4260 ppm for 18.5, 23.3 and 25.6 vol.% metallic powder, respectively). For anisotropic samples, increasing the metal content resulted in higher magnetostriction (2790, 3780 and 4170 ppm for 9.2, 18.5 and 23.3 vol.% metallic powder, respectively). Moreover, the origin of such different behavior will be discussed on this work. The magnetization as a function of the magnetic field ( $H$ ) was performed using superconducting quantum interference device (SQUID) magnetometer. The results shows that magnetization rises linearly with increasing particle content both in isotropic and anisotropic MREs. At higher particle volume fraction,  $M_s$  becomes progressively larger (95 to 167 and 101 to 160 emu/g for 9.2 and 25.6 vol% for isotropic and anisotropic, respectively). Considering that the  $M_s$  of the Hiperco (bulk sample) was 240 emu/g, the results imply that the magnetic contribution originates from the magnetic loading and is not affected by PDMS. The negligible difference in coercive field ( $H_c$ ) for all MREs ( $15.7 \pm 2.6$  Oe) representing that  $H_c$  mainly relies on the coercivity of the particles, regardless of their concentration and direction in matrix.

## Acknowledgements

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# Performance optimization of triboelectric nanogenerators

**Carlos Callaty<sup>1</sup>, Isabel Gonçalves<sup>1</sup>, Cátia Rodrigues<sup>1</sup>, João Ventura<sup>1</sup>**

<sup>1</sup>IFIMUP and Department of Physics and Astronomy, University of Porto, Portugal, carlos.callaty@gmail.com

Triboelectric nanogenerators (TENG) are a promising and attractive energy harvesting technology because of being environmentally friendly, low cost and low maintenance. TENGs allow mechanical energy to be converted into electrical energy in many configurations like the contact separation, sliding, single electrode and freestanding layer modes. The focus of this work is the contact separation mode, where two materials of opposing charge tendencies, with their respective electrode, can be seen as a variable parallel plate capacitor. The contact separation mode converts energy with one of the materials moving and periodically coming in contact with the other material in a fixed position, creating electrostatic charges (triboelectric effect). The motion of the moving material originates a distribution of charge in the electrodes due to the created electrostatic charges present on the materials. Here, we will first present an optimization of the performance of polymer-polymer TENGs through numerical simulations using a finite method. The parameters to be optimized include the area, thickness and permittivity of the TENG materials. To evaluate the performance of the TENG, the open circuit voltage, short circuit voltage were obtained. For the relative permittivity study, we compared the effect of nanoparticle-doping on the contact separation mode TENG. The results obtained are in agreement with the available physical models for the short circuit current. The current increases (decreases) with the increase of the area (thickness of the material) of the TENG. The optimum resistance decreases (increases) with the increase of the area (thickness of the material) of the TENG. The open circuit voltage was found to be constant with the area and the thickness of the material. We will then present a study on the temperature dependence of the TENG performance of the PDMS/Cu,Al structure. We observe that, with the increase of the temperature, the open circuit voltage decreases.

## Acknowledgements

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# IN SILICO MODELING OF PROTRUSION INVASION IN SPHEROIDS

**T. C. Rebocho<sup>1,2</sup>, C. S. Dias<sup>1,2</sup>, N. A. M. Araújo<sup>1,2</sup>**

<sup>1</sup>Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal  
email: csdias@fc.ul.pt

<sup>2</sup> Centro de Física Teórica e Computacional, Universidade de Lisboa, 1749-016 Lisboa, Portugal

Protrusions are an essential process to metastasis. In this process, the cells elongate to optimize the migration capacity. This is driven by mechanical forces between cells and the extracellular environment. The cellular migratory dynamics evolves several biophysical mechanisms. Caballero et al. [1] used cell spheroids to study the dependence of the invasion potential on the frequency of probing, the stability lifetime, and the probing distance of protrusions. Other experiments indicate that cell motility and ECM collagen density are relevant parameters to study different migratory phenotypes [2].

We propose a model and perform numerical simulations to study how cell metastasis depends on the force of protrusions and the dimension of the spheroid. We model cell spheroids as clusters of spheres connected by elastic springs in a viscous medium, and protrusions by random forces applied to a cell. We focus on how the invasion probability is affected by the structure and size of the spheroid. Furthermore, we study how cell-cell and cell-ECM interactions correlate with the lifetime and size of protrusions.

## Acknowledgements

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# DESIGN AND IMPLEMENTATION OF CRYOGENIC CAMARA FOR THERMOELECTRIC DEVICES EVALUATION FOR NANOSATELITES

**R. S. Costa,<sup>1</sup> F. Carpinteiro,<sup>1</sup> M. M. Maia,<sup>1</sup> A. M. Pereira<sup>1</sup>**

<sup>1</sup> IFIMUP, Department of Physics and Astronomy, Faculty of Sciences, University of Porto, Porto, Portugal  
email: [rucosta@fc.up.pt](mailto:rucosta@fc.up.pt)

The CubeSats Era is revolutionizing space exploration field in the last years. Several areas, such as weather information, space weather, transportation, navigation and security, are evaluating to resort to this technology. The CubeSat market generated \$143.7 million in 2017 and is estimated to grow at a CAGR of 13.43% during 2018-2023 [1]. The powering of the CubeSat systems relies on larger solar arrays that still present some limitations such as low efficiency on non-illuminated areas as well as weight problems. Thus, our team purposed an innovative wireless power device using Thermoelectric Generators arrays combined with a laser and a specific absorber allowing a Wireless Energy Transfer (WET) [2]. Since CubeSats are exposed to continuous temperature changes, e.g., due to changing sun irradiation during orbits, and for materials to be suitable for space applications, their performance under thermal cycling in vacuum must be validated.

Herein, the design and implementation of a vacuum cryogenic chamber for performance evaluation of the HPTP as well as validation of the robustness of all components is presented. The cryogenic chamber presents a rectangular-shape being its walls made of an aluminum alloy. The HPTP positioned inside of the cryogenic chamber is thermal stimulated by a laser that cross an optical glass. The output of the HPTP is recorded over the time decreasing/increasing the inside temperature of the chamber from 100 to 400 K (vice-versa).

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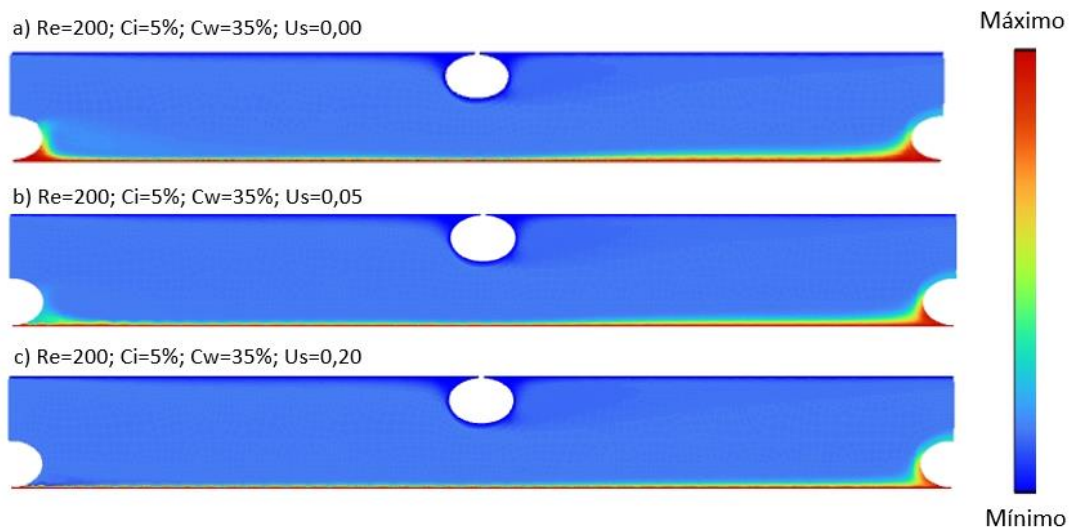
# EFEITO DA VELOCIDADE DE DESLIZAMENTO NA HIDRODINÂMICA NUMA MEMBRANA DE DESSALINIZAÇÃO

A. Morais<sup>1</sup>, Armando A. Soares<sup>1,2</sup>

<sup>1</sup>ECT/UTAD - School of Science and Technology, University of Trás-os-Montes e Alto Douro, Vila Real, Portugal. email: maandrade@utad.com; asoares@utad.pt;

<sup>2</sup>EES-INEGI/LAETA, Institute of Science and Innovation in Mechanical and Industrial Engineering, Porto, Portugal.

Neste trabalho, usaram-se técnicas de Dinâmica dos Fluidos Computacional (CFD), para estudar a hidrodinâmica em canais de alimentação de uma membrana semipermeável de dessalinização com espaçadores dispostos em ziguezague e transversais ao escoamento. As soluções numéricas foram obtidas através de simulações realizadas com o software FLUENT, para escoamentos laminares em canais preenchidos com filamentos. Foi investigada a hidrodinâmica para o regime de escoamento estacionário com e sem deslizamento na parede inferior. Neste estudo apresentamos a distribuição das velocidades, as isolinhas da função corrente, a queda de pressão, as tensões de corte nas paredes, a distribuição da concentração de soluto (NaCl) para diferentes números de Reynolds ( $50 \leq Re \leq 300$ ). Os resultados, para uma célula, mostram que considerando uma velocidade de deslizamento na parede inferior, a velocidade de deslizamento favorece a acumulação de soluto a jusante junto do espaçador. Por outro lado, a montante junto ao espaçador acumula-se menos concentração de soluto. A velocidade de deslizamento resultou num aumento significativo da tensão máxima de corte na parede inferior ao longo da membrana atrasando o início da formação de incrustações. A figura 1 mostra a distribuição da concentração de soluto ao longo da célula com e sem deslizamento na parede inferior considerando  $Re=200$ , concentração de soluto na entrada da célula  $C_i=5\%$  e na parede da célula  $C_w=35\%$ .



**Figure 1.** Distribuição da concentração numa célula para  $U_s= 0, 0,05$  e  $0,2$ .

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# MODELING THE MECHANICAL PROPERTIES OF COLLOIDAL GELS

**João Neves<sup>1,2</sup>, Cristóvão Dias<sup>1,2</sup>, Nuno Araújo<sup>1,2</sup>**

<sup>1</sup> Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal

<sup>2</sup> Centro de Física Teórica e Computacional, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal

email: [fc51402@alunos.fc.ul.pt](mailto:fc51402@alunos.fc.ul.pt)

The identification of the necessary conditions for the emergence of elasticity in a gel is among the most fundamental challenges in gelation. Recent confocal microscopy experiments of colloidal gels suggest that metastability emerges when particles with at least six neighbors percolate [1]. Recently, we found that for particles with limited valence and directional interactions, the onset of elasticity coincides with percolation of particles with three or more neighbors. This result gives support to the percolation of the local isostatic environment as the necessary condition for mechanical metastability and provides insight into the elasticity of low-valence colloid gels. However, it is not clear how bending energy affects the onset of mechanical stability. The scope of this work is to extend the previously developed model to vary the bending energy up to the limit of mobile linker on the surface of each particle. We discuss the effect of the bending energy on the mechanical properties of the gel. These numerical simulations also provides us with valuable information on the mechanical stability of the gel. The transition frequency at which the material becomes predominantly elastic is studied using oscillatory rheology. In addition to this technique, conventional passive microrheology, using mean-square-displacement, and two-point microrheology [2] were also used.

## Acknowledgements

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# JARDIM BOTÂNICO DA UTAD: UM RECURSO EDUCACIONAL E INTERDISCIPLINAR

**A. Andrade<sup>1</sup>, Armando A. Soares<sup>1,2</sup>**

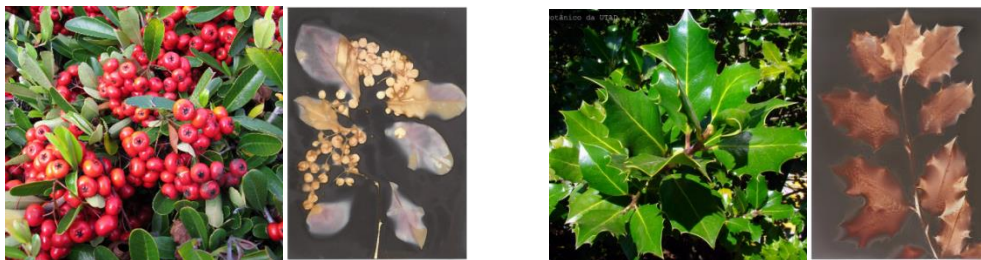
<sup>1</sup>ECT/UTAD - School of Science and Technology, University of Trás-os-Montes e Alto Douro, Vila Real, Portugal. email: aandrade@utad.com; asoares@utad.pt;

<sup>2</sup>EES-INEGI/LAETA, Institute of Science and Innovation in Mechanical and Industrial Engineering, Porto, Portugal.

Com este trabalho pretendemos recuperar um processo fotográfico sem câmara que remonta ao início do aparecimento da fotografia. Este processo fotográfico designado por “Lumen print” foi popularizado pelo fotógrafo americano Jerry Burchfield (1947-2009) ao designar assim as imagens de plantas e flora nativa da floresta amazónica obtidas por este processo.

A qualidade das fotografias obtidas sem câmara depende de vários fatores, entre os quais destacamos; o material de impressão, as amostras botânicas (plantas, folhas e flores, entre outras) recolhidas, a luz, as condições atmosféricas e o tempo de exposição à radiação solar. Dependendo das condições mencionadas as imagens resultantes podem não fornecer muitos detalhes descritivos, tornando difícil a identificação das amostras no seu habitat natural.

Do ponto de vista artístico as imagens obtidas são únicas e podem ser utilizadas em trabalhos práticos de ciências físicas e biológicas, promovendo a interdisciplinaridade entre diferentes áreas do conhecimento. Neste trabalho explicamos o processo de obtenção das imagens do ponto de vista Físico-químico [1, 2]. As imagens obtidas são de espécies pertencentes ao Jardim Botânico da UTAD. Com este trabalho também pretendemos dar início à construção de um herbário com a catalogação de espécies orgânicas do Jardim Botânico da UTAD através deste processo. A figura 1 mostra duas imagens obtidas com o processo fotográfico designado por “Lumen print”.



**Figure 1.** Fotografias e “Lumen print” das espécies *Pyracantha Coccínea* e *Ilex Aquifolium*.

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# HORIZONTAL TEMPERATURE GRADIENTS DETECTION WITH SELF-POWERED THERMOELECTRIC SENSOR

Miguel Almeida,<sup>1</sup> Ana Pires<sup>1</sup>, André Pereira<sup>1</sup>

<sup>1</sup>IFIMUP, Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal  
email: miguelalmeida2199@gmail.com

Thermoelectric devices (TE) have been studied to produce electrical power from a temperature gradient [1]. Thermal sensors are other applications based on the characteristic Seebeck effect of this type of materials. Accordingly, TE materials have a well-defined Seebeck coefficient,  $S = -\Delta V/\Delta T$ , so, through the analysis of the potential difference generated by the material,  $\Delta V$ , it is possible to determine the corresponding temperature variation,  $\Delta T$ . Combining these materials advantages, it is possible to create self-powered sensors [2].

One of the issues in using TE materials as temperature sensors is the need to analyze the potential generated at the temperature variation point, which leads to the need to measure several signals, if the objective is to monitor a large area. Thus, the aim of the present work is to produce a new flexible network configuration that allows the detection of temperature gradients in the horizontal plane to the sensor, using  $N$  stripes of *p-type* TE material transverse to  $N$  stripes of *n-type* TE material. This configuration allows measuring  $4N+N^2$  points in a square area, using only  $2N$  signals.

Firstly, will be introduced the numerical results obtained from a simulation in *Comsol Multiphysics*® for 1X1 and 3X3 networks, which allow the analysis of 5 and 21 distinct points, using 2 and 6 signals, respectively. For the 1X1 network it was possible to obtain sensitivities of 127 and 150  $\mu\text{V K}^{-1}$ , and for the 3X3 network, sensitivities between 14 and 176.6  $\mu\text{V K}^{-1}$ .

Experimentally, *p-type* and *n-type*  $\text{Bi}_2\text{Te}_3$  flexible TE films were printed using the screen-printing technique on kapton substrate, subsequently to the optimization of the TE inks. These inks are composed of commercial TE powder and Poly(vinyl alcohol) doped with phosphoric acid (PVA/ $\text{H}_3\text{PO}_4$ ). The concentrations between PVA and  $\text{Bi}_2\text{Te}_3$  were optimized herein in order to have the highest possible Seebeck coefficient, as well as the best Power Factor ( $\text{PF}=S^2\sigma$ ,  $\sigma$  = electrical conductivity), which describes the capability of energy conversion by the material. For the *p-type* material, the values obtained was  $S$  of 150  $\mu\text{V K}^{-1}$  and PF of 0.33  $\mu\text{W K}^{-2}$ , and  $S$  of -156  $\mu\text{V K}^{-1}$  and PF of 0.75  $\mu\text{W K}^{-2}$  for the *n-type*.

Using the flexible printed sensors, different temperature differences were applied that allowed to confirm the numerically obtained results. In this way, the entire production of the sensor will be discussed and compared with the numerical simulations.

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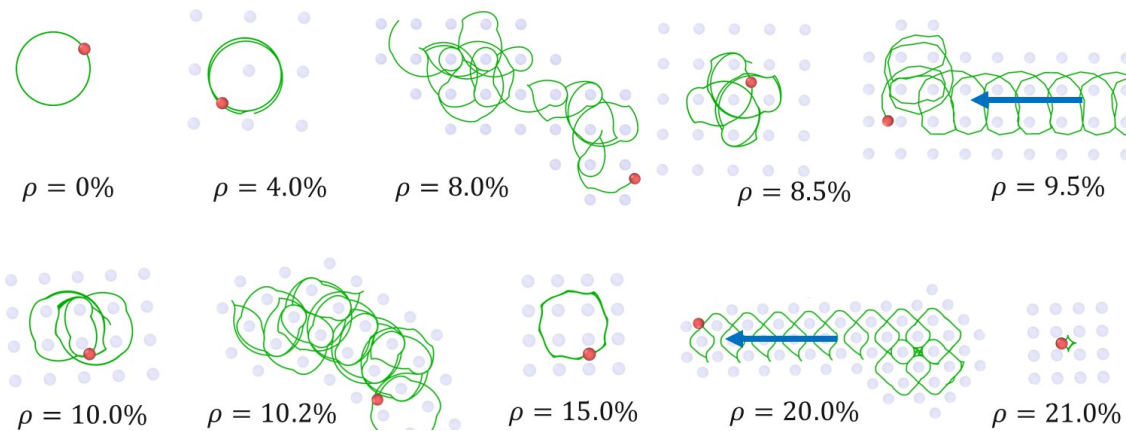
# THE ROLE OF DISORDER IN THE MOTION OF CHIRAL SWIMMERS IN THE PRESENCE OF OBSTACLES

**Danne van Roon,<sup>1</sup> Giorgio Volpe<sup>2</sup>, Margarida M. Telo da Gama<sup>1</sup> and Nuno A.M. Araújo<sup>1</sup>**

<sup>1</sup>Centro de Física Teórica e Computacional, Faculdade de Ciências, Universidade de Lisboa, P1-1749-016 Lisboa, Portugal. E-mail: dvroon@fc.ul.pt

<sup>2</sup>Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK.

The presence of obstacles is intuitively expected to hinder the diffusive transport of micro-swimmers. However, for chiral micro-swimmers, a low density of obstacles near a surface can enhance their diffusive behavior, due to the rectification of the chiral motion by the obstacles. Here, we study numerically the role that disorder plays in determining the transport dynamics of chiral micro-swimmers on surfaces with obstacles. We consider different densities of regularly spaced obstacles and distinct types of disorder: noise in the dynamics of the micro-swimmer, quenched noise in the positions of the obstacles as well as obstacle size polydispersity. We show that, depending on the type and strength of the disorder, the presence of obstacles can either enhance or hinder transport, and discuss implications for the control of active transport in disordered media [1].



**Figure 1.** Example trajectories (green) of the swimmer (red) navigating the square lattice of obstacles (faint blue) for increasing obstacle densities. The blue arrows indicate the direction of propagation of the 'translating orbits'.

We acknowledge financial support by the European Commissions Horizon 2020 research and innovation program under the Marie Skłodowska-Curie Grant Agreement No. 812780 and from the Portuguese Foundation for Science and Technology (FCT) under Contracts no. PTDC/FIS-MAC/28146/2017 (LISBOA-01-0145-FEDER-028146), UIDB/00618/2020, and UIDP/00618/2020.

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# TUNING THE TRANSPORT PROPERTIES OF BiSbTe/PEDOT:PSS/PVA

Inês Ornelas<sup>1</sup>, Margarida Maia<sup>1</sup>, Miguel Almeida<sup>1</sup>, Mariana Rocha<sup>1</sup>, Ana L. Pires<sup>1</sup>, André M. Pereira<sup>1</sup>

<sup>1</sup>IFIMUP, Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal  
email: up201706561@up.pt

Flexible devices composed of thermoelectric (TE) materials can produce electrical power when a temperature gradient is applied. Due to their ability to operate as a distant energy generator, flexible TE technologies have a promising future in our energy-dependent world. Furthermore, TE generators are scalable and easily manufactured employing printing techniques such as screen-printing, which was engaged herein [1].

Under this work, ternary inks composed of PEDOT:PSS (poly(3,4-ethylenedioxythiophene) polystyrene sulfonate), PVA (Poly(vinyl alcohol)) doped with phosphoric acid and BiSbTe (p-type) are being developed and optimised in order to improve the efficiency of the produced devices.

The weight percentages (wt %) of each of the components, i.e. organic and inorganic, is being adjusted thus creating different ink formulations. The studied weight percentages range between 60wt % to 80wt % for Bi<sub>2</sub>Te<sub>3</sub> and 5wt % and 30wt % for the polymers PVA and PEDOT:PSS. This enables us to assess the influence of each of the components in the ternary ink on the transport properties of our devices.

Additionally, the resulting films were fully characterised in terms of their morphology, structure, and transport properties (through its Seebeck coefficient (S) and electrical ( $\sigma$ ) and thermal (k) conductivity). The TE performance is characterised by the figure-of-merit  $ZT=S^2 \times \sigma / k$  and power factor  $PF=S^2 \times \sigma$  [2]. The results obtained from the developed inks showed a higher S and  $\sigma$  for 70wt% of TE, 25wt% of PVA and 5wt% of PEDOT:PSS. Moreover, optimisation surrounding the optimal wt% has been conducted, yielding a PF of approximately 5.14  $\mu\text{W}/\text{K}^2$ . This is an improvement over previous results, where some formulations presented a PF surrounding 0.03  $\mu\text{W}/\text{K}^2$ .

Furthermore, radial flexible TE devices embedded with the foremost ink were manufactured and characterised in a homemade setup that allows low pressure and low-temperature settings under laser incidence. The complete characterisation of the printed films and devices will be presented and thoroughly discussed. The implementation of absorbers in the devices is an objective of the present work.

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# ELECTRONIC TATTOOS FOR MONITORING VITAL SIGNS

**Francisco Mesquita,<sup>1</sup> Ana Pires<sup>2</sup>, André Pereira<sup>3</sup>**

<sup>1</sup> Instituto de Física dos Materiais da Universidade do Porto, Faculdade de Ciências da Universidade do Porto  
email: up201504536@edu.fc.up.pt

<sup>2</sup> Instituto de Física dos Materiais da Universidade do Porto, Faculdade de Ciências da Universidade do Porto

<sup>3</sup> Instituto de Física dos Materiais da Universidade do Porto, Faculdade de Ciências da Universidade do Porto

Biotechnological developments shift medicine from a reactive approach to a more proactive and preventive attitude. Therefore, wearable electronic devices integrated into the skin to monitor health have attracted interest. Electronic tattoos (also known as e-tattoos) — which are stretchable, ultrathin, and ultrasoft membranes — track multiple vital signs and biomarkers [1]. To achieve outstanding performance, these devices must also meet specific criteria regarding design, materials, and fabrication. For health monitoring, the optimal design is an in-plane serpentine shape, which displays an elastic behavior similar to the epidermal layer, notably regarding their extensibility. Thus, a homogeneous deformation followed by a constant electrical conductivity is observed. The materials should be biocompatible, conductive, and skin adherent [2].

In the present work, a serpentine-shaped shadow mask is being used to produce the e-tattoos, in flexible substrates, such as Kapton® polyimide or Polyethylene Terephthalate (PET) films, and a commercial transfer paper tattoo. Screen-printing is the main fabrication used. In the screen-printed electrodes, with approximately 10 µm of thickness, commercially available silver ink has been used.

The characterisation procedures used to investigate the materials and the samples are also being performed. Concerning the structural and morphological characterisation, direct and indirect thickness measurement techniques, Scanning Electron Microscopy (SEM), Electron Dispersive X-Ray Spectroscopy (EDS), and X-Ray Diffraction (XRD) have been implemented. Additionally, the characterisation by their transport properties is being carried out, such as the LRC Impedance Bridge for impedance measurements or the 4-contact method for conductivity measurements. In terms of vital signs monitoring, electrocardiogram (ECG) has been performed through electrodes on the AD8232 Heart Rate monitor, where the captured signal is analyzed by an Arduino algorithm.

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# DEVELOPMENT AND OPTIMIZATION OF BISMUTH TELLURIDE NANOPlates FOR THERMOELECTRIC DEVICES

**Isabel Sousa<sup>1\*</sup>, M. Margarida Maia<sup>\*</sup>, Ana L. Pires<sup>\*</sup>, Mariana Rocha<sup>\*</sup>, André M. Pereira<sup>\*</sup>**

<sup>1</sup>up201605951@edu.fc.up.pt

<sup>\*</sup> IFIMUP – Instituto de Física de Materiais Avançados, Nanotecnologia e Fotónica, Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal

The growing quest for new, improved and sustainable ways to harvest energy and the unprecedented expansion of the Internet of Things (IoT) market keeps pushing technology to the limit nowadays. In 2021 IoT counted with more than 10 billion active devices, however, this number is expected to surpass 25.4 billion by 2030. Despite that, their expansion has been slowed down by the lack of viable power supply methods capable of replacing the old wires or batteries. The latter has several drawbacks such as the requirement of manual maintenance, a finite lifespan, and possible safety risks and environmental harm. [1].

Thermoelectricity is a viable route to solve this problem because it is noiseless, vibrationless, does not produce pollutants, uses waste heat, and has reliable conversion. Thermoelectric materials convert thermal energy into electrical energy through the temperature difference-induced separation of positive and negative charges generating a voltage inside it. However, materials have a low output at ambient operating temperature, so strategies are needed to increase their efficiency. Inside the thermoelectric materials, 2-dimensional (2D) nanostructures present a boost comparing with bulk materials due to quantum confinement effects on the thermal conductivity [2].

This work reports the synthesis and enhancement of Bismuth Telluride ( $\text{Bi}_2\text{Te}_3$ ) nanoparticles, as well as the material structural and morphological characterization (by X-Ray diffraction, scanning electron microscopy, and transmission electron microscopy), and transport properties (electrical conductivity and Seebeck coefficient). The enhancement has performed by studying the variation of the concentration of ethylene glycol and 1-Amino-2-Propanol in its synthesis [3].

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# RASTREABILIDADE EM MEDIÇÕES COM SONDAS DE CONTACTO

**Fernanda Saraiva**,<sup>1</sup> **Carlos Pires**,<sup>2</sup> **Pedro Neves**,<sup>3</sup> **João Alves e Sousa**,<sup>4</sup>

<sup>1,2,3,4</sup>Instituto Português da Qualidade, Rua António Gião, 2, 2829-513 CAPARICA, Portugal  
email: fsaraiva@ipq.pt

O acabamento superficial e a forma dos produtos são características importantes a serem examinadas para fins científicos e de engenharia. Tais características de superfície incluem a resistência ao desgaste, propriedades de rolamento, de deslizamento e de lubrificação, resistência à fadiga e à corrosão, brilho, pintura, funcionalidade, etc. Estes são parâmetros importantes para as indústrias de fabricação de equipamentos e produtos [1].

Para desenvolver processos de medição das características de superfície, que sejam rastreáveis e económicos, o IPQ investiga a utilização de geradores de deslocamento portáteis para calibrar instrumentos com sondas de contacto (*stylus e probes*), a partir da calibração de padrões de forma e de rugosidade, com incertezas de calibração na faixa de 10 nm – 100 nm.

O comportamento de um gerador de deslocamento [2], para determinação das suas propriedades metrológicas, dos seus desvios e estabilidade faz parte do estudo no âmbito do projeto internacional ProbeTrace [3] do programa Europeu EMPIR onde, com a colaboração dos laboratórios de metrologia congéneres ao IPQ e parceiros deste projeto é desenvolvida uma comparação interlaboratorial que visa a determinação dos erros a longo prazo, que possam resultar do transporte deste tipo de padrões entre laboratórios e a identificação de fontes de incerteza de medição e o tratamento estatístico associado.

Na comunicação serão apresentadas as necessidades metrológicas que levaram ao estudo e o desenvolvimento realizado para a implementação de novos métodos de calibração de equipamentos de medição de forma e rugosidade que garantam a sua rastreabilidade metrológica ao metro (unidade de comprimento do SI).



**Figure 1.** Máquina de defeito de forma e de rugosidades (foto IPQ) com sondas de contacto para caracterização de forma das superfícies e determinação dos parâmetros de rugosidade.

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# YOUNG MINDS LISBON

**D. Verheij<sup>1,2</sup>, D. M. Esteves<sup>1,2</sup>, D. R. Pereira<sup>1,2</sup>, M. C. Sequeira<sup>2\*</sup>**

<sup>1</sup> INESC MN, Rua Alves Redol, 9, 1000-029 Lisboa, Portugal

<sup>2</sup> IPFN, Instituto Superior Técnico, Av. Rovisco Pais, 1, 1049-001 Lisboa, Portugal

\* current affiliation: HZDR, Bautzner Landstraße 400, 01328 Dresden, Germany

email: [ymlisbon@ctn.tecnico.ulisboa.pt](mailto:ymlisbon@ctn.tecnico.ulisboa.pt)

The Young Minds Lisbon section was founded in June 2019 by students and researchers from Instituto Superior Técnico of the University of Lisbon — Dirkjan Verheij, Dr. Marco Peres, Daniela Pereira and Dr. Przemysław Józwik. Currently, the Lisbon section is composed of Dirkjan Verheij, Duarte Esteves, Daniela Pereira and Dr. Miguel Sequeira.

Over the last three years, this section has been actively involved with several activities, focusing on outreach and professional development events. In this context, our section has taken part in large-scale events promoting science and research, such as the European Researchers' Night or our home institution open day (Técnico Day). Moreover, we have also organised two successful editions of our flagship event — the Young Minds' Movie Night [1,2]. These events consist of the screening of a movie (e.g., a sci-fi film or a documentary related with Physics), followed by a light presentation on the topic of the movie given by a specialist. This is a fun way to bring Physics to a broader audience and raise awareness on its importance amongst the general public. Additionally, our section has also organised an event named Mental Health @ Técnico, with the goal of discussing several topics related with the importance of the mental wellbeing in the context of the academic environment [3].

In short, the work developed by the Young Minds Lisbon chapter is actively contributing towards the goal of spreading awareness in Physics amongst the general public, with a particular emphasis in the younger generations.

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# HYBRID THERMOELECTRIC-BASED INNOVATIVE SYSTEM FOR WIRELESS ENERGY TRANSFER

**M. M. Maia<sup>1</sup>, A. L. Pires<sup>1</sup>, M. Rocha<sup>1</sup>, A. M. Pereira<sup>1</sup>**

<sup>1</sup>IFIMUP - Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Faculdade de Ciências da Universidade do Porto, 4169-007 Porto, Portugal,  
e-mail: [m.margarida.maia@fc.up.pt](mailto:m.margarida.maia@fc.up.pt)

In an era where mobility and sustainability are high-priority factors to take into consideration in technology development, the concepts of Wireless Energy Transfer (WET) and Energy Harvesting (EH) are gaining exponential interest [1]. Thus, we present an innovative system that combines these two fields, where a thermoelectric device (EH) is powered by a high-power laser (WET).

A radial flexible thermoelectric generator was developed, in which a high-power laser is focused in the centre, creating a temperature gradient, thus generating a voltage. With sustainability in mind, we selected a low-cost and straightforward manufacturing process to fabricate the devices - screen-printing. Commercial silver ink was used for the electrical contacts. The TE ink was developed with a base of a polymer matrix of PVA (Polyvinyl Alcohol) doped with phosphoric acid (16.4 wt%), mixed with PEDOT:PSS (poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate)) (16.4 wt%), and combined with commercial Bi-Te microparticles (67.2 wt%), adapted from a previous study [2]. Transport properties analyses were performed for the printed film. The TE film presents a Seebeck coefficient of  $33 \mu\text{VK}^{-1}$  and electrical conductivity of  $7.32 \text{ Sm}^{-1}$ , thus leading to a Power Factor ( $\text{PF} = S^2\sigma$ ) of  $7.97 \mu\text{Wm}^{-1}\text{K}^{-2}$ .

The characterization of the developed device was performed under vacuum at room temperature, with an incident laser beam with a wavelength of 1450 nm and a variable power (0.5 – 2 W). To increase the generated temperature gradient, a light collector in the centre of the device was considered, and a comparative analysis was carried out. With the collector and a laser power of 2 W, a maximum output voltage of 16 mV and a maximum power density of  $25 \mu\text{Wm}^{-2}$  were achieved. The temperature and pressure effects on the output were also evaluated, and an increase of 25% and 230%, respectively, was observed. This promising technology shows to be a possible alternative for energy generation in remote places.

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# Tuning the optical properties of nanomaterials for buildings façades reflectance improvement

Rita Carvalho Veloso<sup>1,2</sup>, Catarina Dias<sup>1</sup>, Nuno M.M. Ramos<sup>2</sup>, João Ventura<sup>1</sup>

<sup>1</sup>IFIMUP-IN, Departamento de Física e Astronomia, Faculdade de Ciências da Universidade do Porto, Portugal  
email: up201001431@edu.up.pt

<sup>2</sup>CONSTRUCT-LFC, Departamento de Engenharia Civil, Faculdade de Engenharia da Universidade do Porto, Portugal

Nanomaterials can have a significant role in the development and improvement of materials for the construction sector, allowing the design of smart, green and more energy-efficient buildings [1]. One highly appealing solution to improve energy savings in buildings is the application of high reflective finishing coatings, which reduces the surface temperature and consequently decreases the energy required for cooling needs [2]. Due to this, nanomaterials with tuned optical properties, especially metal oxides, can be suitable candidates to enhance the properties of such coatings, improving their reflectivity in the NIR region while at the same time retaining the visual aspect (color) of the conventional coating [3]. Here, we conducted a study of the influence of size, optical band gap energy and concentration of metal oxide nanoparticles (e.g., ZnO, TiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>) dispersed in a conventional black colorant to understand their performance in the visible and near-infrared region (figure 1). The use of the different nanoparticles leads to an important improvement in the total reflectance of the samples. These achievements can lead to the development of innovative envelope systems with increased solar reflectance through new formulations containing metal oxide nanomaterials.

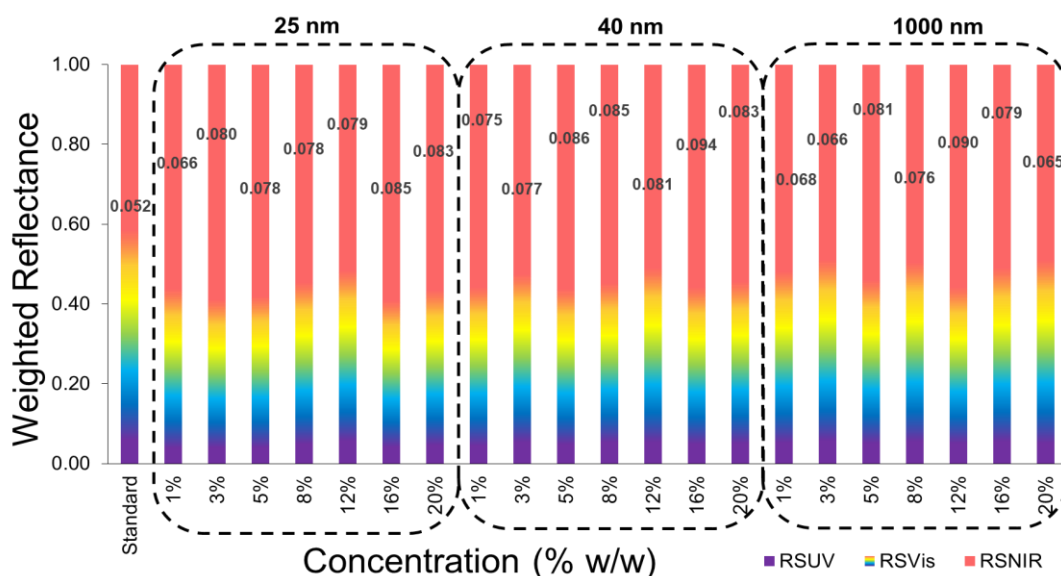


Figure 1. Weighted reflectance calculation of TiO<sub>2</sub> Anatase-doped black colorant.

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# Description of hydrogen atom by a generalized wave equation for $D \geq 3$

Francisco Caruso<sup>1</sup>, Vitor Oguri<sup>2</sup>, Felipe Silveira<sup>2</sup>

<sup>1</sup>Centro Brasileiro de Pesquisas Físicas, Rua Dr. Xavier Sigaud, 150, 22290-180, Urca, Rio de Janeiro, RJ, Brazil

<sup>2</sup> Universidade do Estado do Rio de Janeiro, Rua São Francisco Xavier, 524, 205550-900, Maracanã, Rio de Janeiro, Brazil

email: felipe.silveira@uerj.br

Previously obtained solutions using the  $1/N$  expansion method for the generalization of Schrödinger equation of the hydrogen atom [1], in which the Hamiltonian depends on an iterated Laplacian and a Coulomb-like potential  $r^{-\beta}$  are reviewed and analyzed having focus on the problem of space dimensionality [2]. Consequently, it is shown that new light can actually be shed on the problem of understanding the dimensionality of the world as proposed by Paul Ehrenfest more than a century ago [3]. New results show that not only the sign of the energy but also the values of the ground state energy of the hydrogen atom are both related to the threefold nature of space.

## Acknowledgements

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# DISCUSSÃO SOBRE A MEDIÇÃO QUANTITATIVA DA CRISTALINIDADE EM FILMES ESPESSOS POR ESPALHAMENTO RAMAN

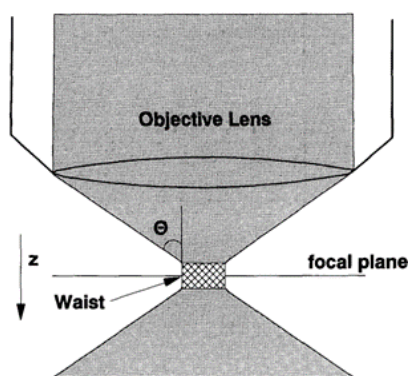
Helena Cristina Vasconcelos,<sup>1,2</sup> Maria Gabriela Meirelles<sup>1</sup>

<sup>1</sup>Universidade dos Açores, Faculdade de Ciências e Tecnologia, Rua da Mãe de Deus, 9500-321 Ponta Delgada, São Miguel, Açores

email: [helena.cs.vasconcelos@uac.pt](mailto:helena.cs.vasconcelos@uac.pt)

<sup>2</sup>Laboratory for Instrumentation, Biomedical Engineering and Radiation Physics (LIBPhys), Lisboa

A medição quantitativa da cristalinidade em filmes espessos por espectroscopia Raman (espalhamento baseada no efeito Raman), tem sido usada com sucesso [1]. Em particular, a  $\mu$ -espectroscopia Raman permite diferenciar e quantificar amostras cristalinas e amorfas. As medições são rápidas, mas a geometria de amostragem tem de garantir que o sinal obtido seja representativo do volume (i.e., da profundidade) e não restrito apenas à superfície. Teoricamente, a intensidade do espalhamento é influenciada por, pelo menos, cinco fatores, independentes dos parâmetros instrumentais, que são: 1. *concentração de fase cristalina*; 2. *tamanho do cristal* que está relacionado ao ordenamento de longo alcance na rede cristalina, e, portanto, à simetria, o que causa um sinal forte [2]. Porém, devido às interações intermoleculares, a simetria de uma molécula no estado cristalino é menor do que num gás (isolado), mas muito maior do que num líquido e no estado amorfo [3]; 3. *arranjo cristalino*. As linhas espectrais de um cristal são função da geometria de espalhamento, ou seja, da orientação recíproca do eixo cristalográfico com o vetor campo elétrico (E) da radiação laser [2]; 4. *múltiplas reflexões* nas amostras policristalinas e 5. *penetração do laser*. O feixe laser exibe o seu menor diâmetro no plano focal da lente, o qual permanece constante até uma certa distância do plano focal [4]. Este elemento de volume é designado por cintura do feixe de laser. O comprimento da cintura ( $w$ ), ou *waist* (profundidade de foco) (Fig.1), pode ser



determinado por [4]:  $w = 6.4 \left( \frac{\lambda}{2\pi} \right) \left( \frac{1}{\tan \theta} \right)^2$ , onde  $\lambda=514$  nm,  $\theta$  é o ângulo definido pela Abertura Numérica ( $NA = \sin \theta$ ). Se o tamanho da cintura for muito pequeno, a análise quantitativa não pode ser realizada visto a distribuição cristalina não homogênea nos filmes, a variação da espessura do filme e o erro operacional contribuirão para grandes variações nos resultados. A metodologia da medição quantitativa foi testada em filmes de  $\text{SiO}_2\text{-TiO}_2$  com dispersão de anatase, produzidos pelo método sol-gel.

Figura 1. Distribuição do feixe laser junto ao foco [4].

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# SURFACE ANALYSIS OF THICK TARGETS BY NUCLEAR TECHNIQUES

**José A. R. Pacheco de Carvalho<sup>1,2</sup>, Cláudia F. F. P. Ribeiro Pacheco<sup>1</sup>, A. D. Reis<sup>1,2</sup>**

<sup>1</sup> APTEL (Applied Physics and Telecommunications) Research Group, <sup>2</sup> Dept. de Física, Universidade da Beira Interior, 6201-001 Covilhã, Portugal  
Contact email: pacheco@ubi.pt

Various complementary techniques have been developed for surface analysis of materials. Nuclear techniques, using low energy MeV ion beams, give absolute values of concentrations of isotopes and elements for a few microns close to the surface. Their main applications have been given in areas such as scientific, technologic, industry, arts, archaeology and medicine [1-7]. Tracing of isotopes with high sensitivities is possible by nuclear reactions. The energy analysis method is used for ion-ion reactions. At a suitable bombarding energy, an energy spectrum is recorded of ions from reaction events occurring at several depths in the target. Such spectra are computer predicted and compared to data, giving target composition and concentration profile information [4-7]. Elastic scattering is a particular and important case of nuclear reactions. A computer program has been developed in this context, mainly for flat targets [4-6]. The non-flat target case arises as an extension. Depth profiling of light nuclei e.g.  $^{12}\text{C}$  is made by the  $^{12}\text{C}(\text{d},\text{p})^{13}\text{C}$  reaction in a thick flat target of extremely high purity pyrolytic graphite. Experimental details are available [4]. The simulations used published nuclear data, namely for differential cross section and stopping power. A very good computed fit was reached to spectral along a high depth of  $X_1 > 12.5 \mu\text{m}$ . The result would be difficult to obtain by other techniques, showing nuclear reaction analysis as a highly powerful analytical tool for non-destructive surface analysis of materials.

Elastic scattering of  $\alpha$  particles was used for analysis. Published nuclear data were used in the simulations. Rutherford and resonant scattering differential cross section were used when applicable. A very good computed fit was obtained to the  $\alpha$  spectrum obtained from a thick flat target containing a compound of Al and O. Elastic scattering has shown to be an additional strong non-destructive analytical tool for surface analysis.

## Acknowledgements

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# SCANNING KELVIN PROBE - CHARACTERIZATION OF SOLID-STATE DEVICES

A. N. Guerreiro<sup>1</sup> and M. Helena Braga<sup>2\*</sup>

<sup>1</sup>Engineering Physics Department, FEUP, University of Porto, 4200-465 Porto, Portugal;  
nguerreiro@fe.up.pt

<sup>2</sup>LAETA-INEGI, Engineering Physics Department, FEUP, University of Porto, 4200-465 Porto, Portugal;

\*Correspondence: mbraga@fe.up.pt;

The socio-economic development of contemporary societies is due to the great technological development of energy production and distribution. This development was at the expense of the consumption of fossil fuels with environmental consequences. The environmental problems created by the use of fossil fuels, force us to rethink the entire paradigm of energy production. Since the beginning of the 21<sup>st</sup> century, we have had a significant investment in the production of electricity from alternative energies. An energy transition is needed to enable sustainable development and a stable electricity supply. In addition to this, we have had a high and fast technological development from mobile phones to biotechnology.

Concerning that, devices like cells and batteries can contribute to that main objective by grouping knowledge from various areas of physics, materials science, electrochemistry, digital technology, and engineering. The study of new materials that can improve and innovate the performance of cells/batteries that are capable and reliable to face the new energy challenges is extremely important. The study of materials for electrodes, and electrolytes, namely, ferroelectric and thermoelectric properties can be translated into a significant advance[1][2]. In that regard, the study of different materials with the Scanning Kelvin Probe (SKP) technique can improve a better understanding of the surface phenomena between different materials like conductors' metals (copper, aluminum, and zinc), dielectrics (oxides), and shell materials like cork. These studies were complemented with Electrochemical Impedance Spectroscopy (EIS) and Cyclic Voltammetry (CV) studies to characterize the electrochemistry of the pair of metals with electrolyte disjoined by an oxide. These studies can guide the choice of material groups for more efficient battery cells.

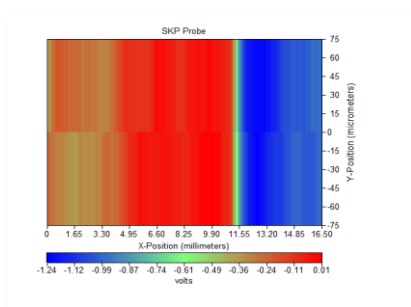


Figure 1. Gradient of the electrical potential of the Cu\_ZnO\_Al obtained by SKP

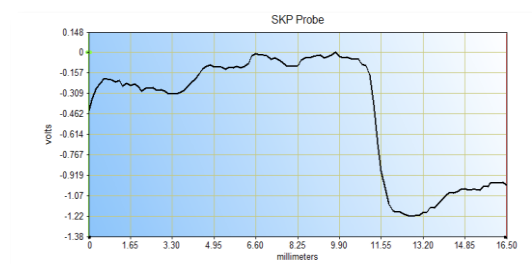


Figure 2. Evolution of the electrical potential of the Cu\_ZnO\_Al obtained by SKP

**Keywords:** Scanning Kelvin Probe; ferroelectric electrolytes; energy storage; electrical conductivity; ionic conductivity; materials science

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# Algorithm for faster and less destructive elemental mapping in Laser Induced Breakdown Spectroscopy

**D. Capela<sup>1,2,\*</sup>, M. F. S. Ferreira<sup>1,2</sup>, A. Lima<sup>3,4</sup>, P. A. S. Jorge<sup>1,2</sup>,  
D. Guimarães<sup>2</sup>, N. A. Silva<sup>2</sup>**

<sup>1</sup> Department of Physics and Astronomy, Faculty of Sciences, University of Porto, Rua do Campo Alegre, Porto, Portugal

<sup>2</sup> INESC TEC, Rua do Campo Alegre, 687, 4150-179 Porto, Portugal.

<sup>3</sup> Department of Geosciences, Environment and Spatial Plannings, Faculty of Sciences, University of Porto, Rua do Campo Alegre, Porto, Portugal

<sup>4</sup> ICT - Institute of Earth Sciences, Faculty of Sciences, University of Porto, Rua do Campo Alegre, Porto, Portugal

\*email: diana.f.capela@inesctec.pt

Laser Induced Breakdown Spectroscopy (LIBS) is a technique that allows fast elemental mapping of sample surfaces. However, to obtain high resolution maps one needs grids with larger number of points, resulting in a time-consuming task and an excessive sample damage. This can be problematic when LIBS is applied in critical areas of industry where quick analyses are crucial for efficiency, or to research of cultural heritage for which the sample damage must be minimized to not spoil the heritage.

In this context, we developed an image-based algorithm for grid optimization using superpixel segmentation (Simple Linear Iterative Clustering – SLIC [1]) to improve the LIBS mapping process. The aim was to produce unstructured grids instead of regular ones, where the mapping points are the centroid of each segmentation zone.

The results obtained show that this approach allows similar accuracy levels for considerably faster mappings when compared with the obtained for regular grids as well as better mapping performances for the same order of grid number of points which translates into a great improvement for this technique.

## Acknowledgments

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# Realtime Classification of Optically Trapped Particles

**Vicente Rocha,<sup>1,2</sup> João Oliveira,<sup>1,2</sup> Pedro A. S. Jorge,<sup>1,2</sup> Ariel Guerreiro,<sup>1,2</sup> Nuno Silva<sup>1,2</sup>**

<sup>1</sup>INESC TEC, Centre of Applied Photonics, Rua do Campo Alegre 687, 4169-007 Porto, Portugal

<sup>2</sup> Departamento de Física e Astronomia da Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal

email: [vicentevrocha.vvr@gmail.com](mailto:vicentevrocha.vvr@gmail.com)

Optical tweezers[1] use highly focused beams of light to trap and manipulate mesoscopic sized transparent particles. Furthermore, the acquisition of the forward scattered beam by a quadrant photodetector allows the precise tracking of trapped particles allowing the study of Brownian motion. As is known, Brownian dynamics depend on both particle and surrounding medium properties making the position a valuable source of information. Recent studies have demonstrated the possibility for machine learning methods for classification of particles using the forward scattered signal[2]. Nevertheless, these methods require the determination of static properties of the particle possible only through position timeseries with long acquisition times. In this work, we exploit the possibility for the application of Recurrent Neural Networks (RNN), namely Reservoir Computing (RC)[3], for the realtime classification of trapped particles. Our dataset consists of experimental position timeseries of Polystyrene (PS) and Polymethylmethacrylate (PMMA) with distinct sizes. In a series of cross-validation routines we test the classification capability of ESN in subgroups of same sized particles with different types or different sized particles with same type. In conclusion, the realtime classification of particles represents a step towards fast and intelligent microfluidic devices with interest in a plethora of natural sciences.

## Acknowledgements

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# PRESSURE-INDUCED PHASE TRANSFORMATIONS OF Sr<sub>3</sub>Hf<sub>2</sub>O<sub>7</sub>

**M. C. B. Barbosa**<sup>1\*</sup>, **E. Lora da Silva**<sup>1</sup>, **P. Neenu Lekshmi**<sup>1</sup>, **Michel L. Marcondes**<sup>2</sup>,  
**Lucy V. C. Assali**<sup>2</sup>, **Helena M. Petrilli**<sup>2</sup>, **A. M. L. Lopes**<sup>1</sup>, **J. P. Araújo**<sup>1</sup>

<sup>1</sup> IFIMUP, Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Department of Physics and Astronomy, Faculty of Sciences, University of Porto, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal

<sup>2</sup> Instituto de Física, Universidade de São Paulo, Rua do Matão 1371, São Paulo 05508-090, Brazil

\*up201506005@edu.fc.up.pt

We present an *ab-initio* study performed by means of Density Functional Theory (DFT) and lattice dynamics to probe the octahedral distortions, which occur during the structural phase transitions of the quasi-2D layered perovskite Sr<sub>3</sub>Hf<sub>2</sub>O<sub>7</sub> (SHO) compound. Such a system is characterized by a high-temperature *I4/mmm* (space group n. 139) centro-symmetric structure and a ground-state *Cmc2<sub>1</sub>* (space group n. 36) ferroelectric phase. We have probed potential candidate polymorphs that may form the *I4/mmm* towards the *Cmc2<sub>1</sub>* transition pathways [1] from which the lower symmetry structural phases may be generated by inducing tiltings and/or rotations of the O octahedral cages. We mainly focus our attention to the *Ccce* (space group n. 68) structural phase, since it has been experimentally evidenced in systems with similar stoichiometry, i.e. Ca<sub>3</sub>Mn<sub>2</sub>O<sub>7</sub> [2]. This phase may occur through a first-order phase transition when temperature decreases towards room temperature, breaking the center-of-symmetry of the tetragonal phase. By observing the phonon dispersion curves of the *Ccce* phase [1] we find that the system is dynamically unstable at the given conditions of the calculation (0 K and 0 GPa), evidencing negative phonon modes localized at two of the high symmetry points of the Brillouin-zone (BZ):  $\Gamma$ - and Y-points. Thus being, a pressure study was executed and it was verified that the *Ccce* structural phase becomes thermodynamically and dynamically stable at 0K and 20 GPa.

As a continuation of the work done so far in SHO, we will show the evolution of the electronic properties of the *Ccce* phase with increasing hydrostatic pressure and further explore the phonon dispersion curves to determine which vibration modes are Infrared and Raman active. Furthermore, the Quasi-Harmonic Approximation (QHA) will be applied to include the anharmonic effects needed to account for thermal expansion, allowing its calculation along with the heat capacity at each pressure value.

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# PERFORMANCE STUDIES OF IEEE 802.11 AC LABORATORY LINKS

**José A. R. Pacheco de Carvalho<sup>1,2</sup>, Hugo Veiga<sup>1</sup>, Cláudia F. F. P. Ribeiro Pacheco<sup>1</sup>,  
A. D. Reis<sup>1,2</sup>**

<sup>1</sup> APTEL (Applied Physics and Telecommunications) Research Group, <sup>2</sup> Dept. de Física, Universidade da Beira Interior, 6201-001 Covilhã, Portugal  
Contact email: pacheco@ubi.pt

The increasing importance of wireless communications, involving electronic devices, has been widely recognized. Performance is a fundamental issue, resulting in more reliable and efficient communications. Wi-Fi has nominal transfer rates up to 11 (802.11b), 54 Mbps (802.11 a, g), 600 Mbps (802.11n) and 6.9 Gbps (802.11ac) [1]. The medium access control of Wi-Fi is carrier sense multiple access with collision avoidance (CSMA/CA). Security is also crucially important. Studies have been published on wireless communications, wave propagation [2,3], practical realizations of WLANs [4]. Laboratory measurements are presented about several performance aspects of Wi-Fi IEEE 802.11ac WPA2 point-to-point links. Our study leads to performance evaluation of this technology under WPA2 encryption, using available equipment (Cisco 2702i access points and Edimax AC1200, EW-7822UAC, USB 3.0 adapters). New results are presented from a devised solution that uses an experimental setup and method, to monitor signal to noise ratios (SNR) and noise levels (N), and measure TCP throughput (from TCP connections) versus TCP packet size, and UDP jitter and percentage datagram loss (from UDP communications) versus UDP datagram size. In the process of data acquisition, Iperf software [5] is used. The results are obtained in batch mode and recorded as data files to the client PCs disks. The statistical analysis, including calculations of confidence intervals, is done as in [6]. Comparisons are made to results obtained for corresponding IEEE 802.11n links [7]. Conclusions are drawn about the comparative performance of the links.

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# THE INFLUENCE OF THE SOLID ELECTROLYTE SURFACE AREA ON THE ELECTROCHEMICAL PERFORMANCE OF A COAXIAL STRUCTURAL BATTERY

**Mafalda Valente<sup>1,2</sup>, Federico Danzi<sup>3,4</sup>, Nuno Guerreiro<sup>2</sup>, M. Helena Braga<sup>2,3</sup>**

<sup>1</sup>Metallurgical and Materials Engineering Department, Engineering Faculty, University of Porto, R. Dr. Roberto Frias s/n, 4200-465 Porto, Portugal MV email: up201904826@fe.up.pt

<sup>2</sup>Engineering Physics Department, Engineering Faculty, University of Porto, R. Dr. Roberto Frias s/n, 4200-465 Porto, Portugal

<sup>3</sup>LAETA-INEGI, Institute of Science and Innovation in Mechanical and Industrial Engineering, 4200-465 Porto, Portugal

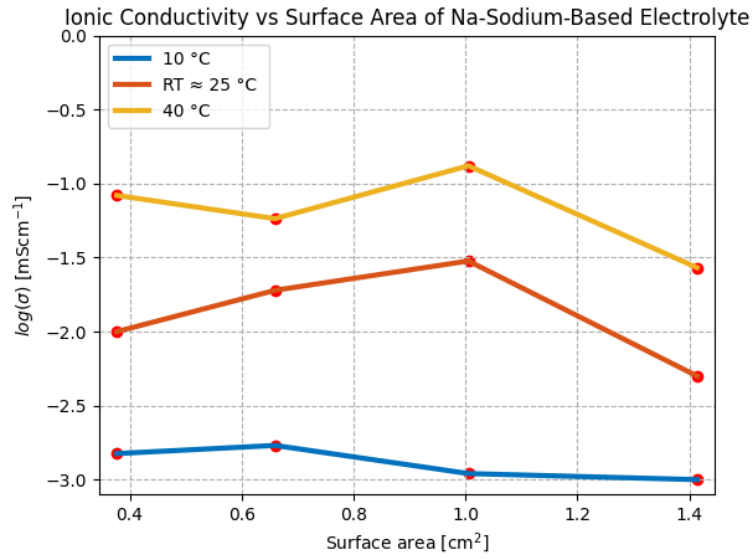
<sup>4</sup>Mechanical Engineering Department, Engineering Faculty, University of Porto, R. Dr. Roberto Frias s/n, 4200-465 Porto, Portugal

corresponding author: mbraga@fe.up.pt

The development of more efficient and sustainable energy storage systems is going to be the key to a greener and safer future. Multifunctional materials capable of working as batteries while bearing mechanical loads show up as one of the most promising options [1]. Within this framework, the new concept of sodium-based all-solid-state coaxial structural battery is here investigated. This innovative design rises intending to optimize the volume of hollow beam-like structures by embedding an all-solid-state battery, eliminating the risks of using a liquid electrolyte and reducing the ecological footprint of traditional lithium-ion batteries. By integrating all-solid-state cells in CFRP cylinders, it is possible to manufacture an electrochemical system that not only can be used to produce energy but also improves the mechanical properties of the final structure [2].

This work aimed to analyze the sensibility of the electrochemical performance in coaxial structural batteries by designing variables such as its geometry. More in detail, the investigated geometrical parameter was the CFRP inner shell diameter, in the Al/ferroelectric- $\text{Na}_{2.99}\text{Ba}_{0.005}\text{ClO}$  composite/Cu electrochemical systems, being the first metal the coaxial electrode and the second the electrode co-cured with the CFRP. The ferroelectric- $\text{Na}_{2.99}\text{Ba}_{0.005}\text{ClO}$  composite is a mixture of 4  $\text{Na}_{2.99}\text{Ba}_{0.005}\text{ClO}$ : 2 Polyvinyl acetate. To assess the performance of the batteries, Electrochemical Impedance Spectroscopy (EIS), Cyclic Voltammetry (CV), and charge/discharge cycles were analyzed. Both EIS and CV were performed at 10°C, RT (approximately 23-25°C) and 40°C. As for the cycles of charge and discharge, they were performed at 40°C.

Moreover, as shown in Figure 1, it was possible to find an optimal radius for different temperatures. At 40°C and RT, the best value of ionic conductivity was observed for the cell with a 6 mm inner radius. Contrary to the trend found for the previous temperatures, at 10°C, the cell that showed higher ionic conductivity was the one with an inner radius of 5 mm.



**Figure 1.** Ionic conductivity vs surface areas for solid-state coaxial cells at different temperatures.

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# COMPOSITE POLYMER ELECTROLYTE PVA/ $K_{2.99}Ba_{0.005}ClO$ FOR STRUCTURAL BATTERIES APPLICATIONS

Maryam Niazi,<sup>1,2</sup> M. Helena Braga<sup>1,2,\*</sup>

<sup>1</sup>Engineering Physics Department, Engineering Faculty, University of Porto, 4200-465 Porto, Portugal; 202103277@fe.up.pt (M.N); mbraga@fe.up.pt (M.H.B)

<sup>2</sup>LAETA-INEGI, Institute of Science and Innovation in Mechanical and Industrial Engineering, 4200-465 Porto, Portugal.

\*Correspondence: mbraga@fe.up.pt

In recent years, many investigations have been performed to achieve more efficient, more sustainable, lighter, greener, and safer types of batteries. In this regard, the design of structural batteries with the capability of carrying mechanical loads and storing electric energy at the same time has been the breakthrough in energy storage. Solid composite polymer electrolytes (SCPEs) with high electrochemical stability and high ionic conductivity are crucial in the development of structural batteries. SCPEs apart from multifunctional by carrying the mechanical load and storing energy at the same time, have other advantages such as no flammability, high-temperature resistance, non-volatilization, and high flexibility, making them interesting for many applications.

Inorganic solid-state ferroelectric oxide electrolytes such as  $K_{2.99}Ba_{0.005}ClO$  have recently shown a high ionic conductivity. However, on the other hand, they still present challenges to overcome including hygroscopicity, and poor interface contact between electrolyte and electrodes. One way to overcome these challenges is to design composite polymer electrolytes.

In this study, composite polymer electrolytes were prepared with  $K_{2.99}Ba_{0.005}ClO$  in polyvinyl alcohol (PVA) blend polymers with different compositional ratios. The pair of electrodes used, Zn (-)//Cu (+) have double function as current collectors, simplifying while reducing the costs even further. The mechanical and electrochemical properties of the cells with different compositional ratios of PVA are examined.

Structural batteries may in the future substitute battery packs if performing as aimed and mitigate the deficit of mechanical equilibrium introduced by heavyweight concentration with the displacement of the centre of mass in vehicles such as autos, bicycles, drones, submarines, and airplanes.

## Acknowledgements

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# OBSERVED GEOMAGNETIC FIELD ANOMALIES AND POSSIBLE CONSEQUENCES

Maria Rosa Duque<sup>1</sup>

<sup>1</sup>Departamento de Física da Universidade de Évora, ECT. Rua Romão Ramalho nº 59, 7000-671 Évora.  
Email: [mrاد@uevora.pt](mailto:mrاد@uevora.pt)

Geomagnetic field data recorded by Magnetic Observatories, located in the Iberian Peninsula, at the end of February 1969, and inserted in Anais of the Observatories referred in the form of average hourly values of the vertical field, horizontal field and magnetic declination [1],[2] were used in the present work. The analysis of the records studied shows the occurrence of identical anomalies in days 26th and 27th but with less amplitude in day 26th. At the end of the great variation occurred on day 27 it is observed in all the Observatories an increase of the vertical component by about 9-10 nT and a decrease of the horizontal component from -35 to -22 nT. The comparison of the values obtained in Coimbra on February 26<sup>th</sup> and 27th shows an increase in the intensity of the field, between hour 10 and hour 15, which is essentially due to an increase in the horizontal component of the field. Another increase was observed, between hours 18 and 20, which is essentially due to an increase in the vertical component of the field. Given that these are variable magnetic fields, we can say that the horizontal component may be associated with ion movement in the vertical direction while the increase of the vertical component of the field may be associated with horizontal movement of ions. If this hypothesis is valid, we could have had, on the 27th, mainly vertical followed by mainly horizontal, ion movements. Between hours 14 and 17 there were large variations in the horizontal component and in the vertical component that led to significant changes in the slope and direction of the field. Thus, we will have electric fields associated with magnetic fields changing in intensity and direction, in an ocean environment.

## Acknowledgements

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# SÉCULO XXI - ASSOCIAÇÃO DAS HABILIDADES NAS ATITUDES E PERCEÇÕES DOS ESTUDANTES EM RELAÇÃO À FÍSICA

Meirelles, M.,<sup>1</sup> Vasconcelos, H. C.<sup>1,2</sup>

<sup>1</sup>Universidade dos Açores, Faculdade de Ciências e Tecnologia, Rua da Mãe de Deus, 9500-321 Ponta Delgada, São Miguel, Açores

email: [maria.gf.meirelles@uac.pt](mailto:maria.gf.meirelles@uac.pt)

<sup>1,2</sup> Laboratory for Instrumentation, Biomedical Engineering and Radiation Physics (LIBPhys), Lisboa

email: [helena.cs.vasconcelos@uac.pt](mailto:helena.cs.vasconcelos@uac.pt)

No século XXI, vivemos num sistema social global, caracterizado pela complexidade, imprevisibilidade e interdependência e por isso são vários os desafios que os países, as instituições, as organizações e os indivíduos em geral terão de enfrentar. Os avanços tecnológicos ocorrem todos os dias. Ser competitivo na era digital implica ser fluente na linguagem em que os avanços tecnológicos operam. Preparar indivíduos com competências que correspondam a estes desafios, é da responsabilidade do sistema educativo. Segundo [1], as competências que os alunos necessitam são o pensamento crítico, a resolução de problemas, a inovação, dimensões estas associadas ao desempenho académico e aos processos de ensino e aprendizagem. O relatório [2], sugere que os professores; i) tornem os conteúdos a trabalhar relevantes para os alunos; ii) “tragam” o mundo exterior para dentro da sala de aula; iii) levem os alunos para fora da sala de aula; iv) criem oportunidades para que os alunos possam interagir uns com os outros, com outros professores e adultos em experiências de aprendizagem significativas. O objetivo do estudo aqui apresentado é, determinar a associação das habilidades no século 21 nas atitudes e perceções dos alunos em relação à Física. De acordo com [3], foi elaborado um questionário que consistiu em colocar a um conjunto de 142 estudantes, uma série de perguntas com respeito a identificar as atitudes em relação à Física e as perceções sobre o ensino e a aprendizagem da Física. A análise dos dados indica que dos estudantes participantes neste estudo: (1) 67,6% têm idades compreendidas entre os 18 e os 21 anos; (2) estão a frequentar o ensino secundário; (3) 71% residem na região Açores. Apresentam uma atitude positiva em relação à Física, 42,2% afirmam que a disciplina de Física consiste em atividades ou projetos que ensinam os estudantes a pensar de forma crítica ou criativa. Do universo da amostra de estudantes, 50% afirmam que os conhecimentos/conceitos adquiridos na Física são utilizados na vida diária. 41,5% dos estudantes inquiridos percecionam que os professores de Física divulgam em sala de aula artigos de ciências ou Física. Menos positiva é a perceção dos estudantes em relação à questão de serem incentivados pelos seus professores de Física a participarem em competições sobre inovação em ciência. Da amostra dos 142 estudantes, apenas 29% afirmaram ter recebido este tipo de incentivo.

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# MAGNETIC CNT-O@MnFe<sub>2</sub>O<sub>4</sub> ELECTRODE NANOMATERIAL: A POWERFUL SOLUTION TO IMPROVE THE ENERGY STORAGE PERFORMANCE OF A SHINY TEXTILE DEVICE

**Joana S. Teixeira,<sup>1,2</sup> André M. Pereira,<sup>2</sup> Clara Pereira<sup>1</sup>**

<sup>1</sup> REQUIMTE/LAQV, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto (FCUP), Rua do Campo Alegre s/n, 4169-007, Porto, Portugal; email: joanafsteixeira@hotmail.com

<sup>2</sup> IFIMUP, Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Department of Physics and Astronomy, FCUP, Rua do Campo Alegre s/n, 4169-007, Porto, Portugal

The design of multifunctional wearable energy storage technologies has been highly requested for high-tech consumers. Carbon-based textile supercapacitors (SCs) are highlighted as an efficient energy storage solution due to their fast charging, high power density and robustness [1]. However, these SCs present limited energy density. The design of electrode materials based on the hybridization of carbon nanomaterials with transition metal oxides (TMO) is a potential strategy to improve such property. Magnetic spinel-type ferrites are a promising option of TMO due to their magnetic properties and diverse oxidation states of the constituting metal cations, endowing an additional pseudocapacitive energy storage mechanism to the device, besides the non-Faradaic electric double-layer phenomenon arising from the carbon component. Glow-in-the-dark pigments are used in textiles, being an auspicious solution to impart dual-functionality to SCs, due to their phosphorescent properties, useful for high-visibility clothing [2].

In this work, a shiny hybrid textile SC that simultaneously exhibits phosphorescent and energy storage properties was fabricated. The high energy storage capability was obtained using textile electrodes coated with a hybrid of oxidized carbon nanotubes and manganese(II) ferrite (CNT-O@MnFe<sub>2</sub>O<sub>4</sub>) and a redox-active phosphorescent solid-gel electrolyte.

The CNT-O@MnFe<sub>2</sub>O<sub>4</sub> was produced by one-pot coprecipitation method, being composed of spherical nanoparticles (cubic spinel structure; crystallite size = 5.5 nm) immobilized on oxidized carbon nanotubes (CNT-O). An asymmetric CNT//CNT-O@MnFe<sub>2</sub>O<sub>4</sub>-IP device was fabricated, which was composed of CNT and CNT-O@MnFe<sub>2</sub>O<sub>4</sub>-coated textile electrodes sandwiching a novel solid-gel electrolyte doped with a redox-active inorganic pigment (IP). For comparison, CNT//CNT and CNT//CNT-O@MnFe<sub>2</sub>O<sub>4</sub> devices based on the undoped electrolyte were prepared. A working potential of 1.36 V was achieved for CNT//CNT-O@MnFe<sub>2</sub>O<sub>4</sub>, leading to an energy density of 8.13 μW h cm<sup>-2</sup> at a power density of 835.8 μW cm<sup>-2</sup>. The synergy between CNT-O and MnFe<sub>2</sub>O<sub>4</sub> led to the simultaneous occurrence of pseudocapacitive and non-Faradaic energy storage mechanisms within the device. The use of IP in the electrolyte of CNT//CNT-O@MnFe<sub>2</sub>O<sub>4</sub>-IP resulted in additional improvements of 30% and 20% in energy density and power density, respectively, relative to CNT//CNT-O@MnFe<sub>2</sub>O<sub>4</sub>. Furthermore, the IP conferred intense green phosphorescence to the textile SC under a dark environment, overcoming the limiting dark color of carbon-based SCs.

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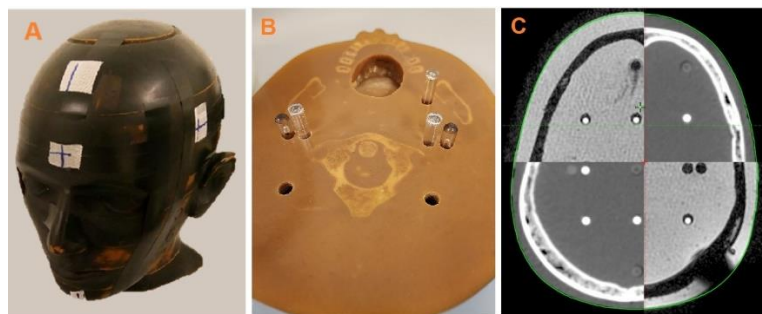
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# OPTIMIZATION OF THE 3T MRI ACQUISITION FOR RADIOSURGERY PATIENTS USING A CUSTOMIZED HEAD PHANTOM

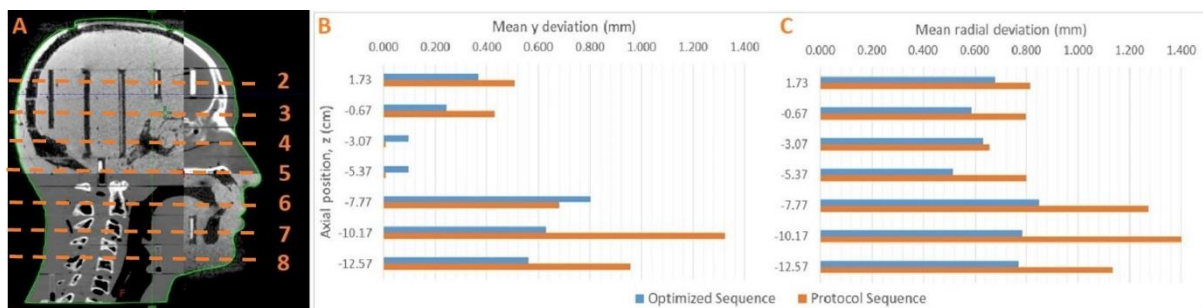
**S. Silva<sup>1,2</sup>, S. Pinto<sup>1,2</sup>, P. Conde<sup>2,3</sup>, J. Lencart<sup>1,2</sup>, E. Machado<sup>3</sup>, J.A.M. Santos<sup>1,2,4</sup>**

<sup>1</sup> Medical Physics Service, Portuguese Oncology Institute of Porto (IPOP), Portugal <sup>2</sup> Medical Physics, Radiobiology and Radiation Protection Group, IPO Porto Research Center (CI-IPOP), Porto, Portugal <sup>3</sup> Department of Imaging Sciences and Radioncology, (IPOP), Portugal <sup>4</sup> Instituto de Ciências Biomédicas Abel Salazar (ICBAS), Porto, Portugal. Email: ssilva23@gmail.com

**Introduction:** Radiosurgery (SRS) treatment planning is based on the delineation of target volumes and organs at risk on MRI scans. Thus, geometric distortion on 3T MRI is a concern as it can lead to an overall increase in treatment delivery uncertainties [1]. **Purpose:** To test a customized phantom to measure MRI distortions and optimize the SRS MRI acquisition protocol. **Methods:** the head of an Alderson Rando® phantom was customized with a total of 48 sealed acrylic inserts (Fig 1-B) filled either with water or gadolinium contrast solution. The tissue equivalent material of the phantom and the natural skeleton inside it [2] provides enough MRI contrast and good registration with CT images (Fig 1-C). Increase of bandwidth from 244 to 781 kHz/pixel and choice of isotropic voxels were tested as recommended [1]. **Results:** Mean coronal (y) deviation of inserts' image is reduced on the optimized acquisition on most but not all the slabs (Fig 2, B). Radial (x,y) distortion is reduced on all slabs (Fig 2, C). **Conclusion:** Although more validation tests are needed, improvement of image quality on MRI 3T for SRS was achieved. The customized phantom is a promising tool to measure distortions on MRI.



**Figure 1.** A: Head of Rando phantom; B: Water filled inserts on a slab; C: Registration of MRI and CT, where the coronal (y) deviation of water inserts on the Protocol MRI is clearly seen.



**Figure 2.** A: Registered MRI and CT, with slab numbers (2-8); slabs 2 and 8 are centered at  $Z=1.73$  cm and  $Z=-12.57$  cm, relative to MRI isocenter. B and C: Mean coronal (y) and radial (x,y) deviations across the phantom slabs, on both acquisition sequences.

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# Field effect transistors on MoO<sub>3</sub> crystals and pseudo-layers: fabrication and characterization

**Daniela R. Pereira<sup>1,2\*</sup>, Chamseddine Bouhafs<sup>1,2</sup>, Sónia O. Pereira<sup>3</sup>, Carlos Díaz-Guerra<sup>4</sup>, Marco Peres<sup>1,2</sup>, António J. S. Fernandes<sup>3</sup>, Bohdan Kulyk<sup>3</sup>, Florinda M. Costa<sup>3</sup>, M. Rosário P. Correia<sup>3</sup>, Eduardo Alves<sup>2</sup>, Susana Cardoso<sup>1</sup>, Paulo P. Freitas<sup>1,5</sup>, Katharina Lorenz<sup>1,2</sup>**

<sup>1</sup>Instituto de Engenharia de Sistemas e Computadores – Microsistemas e Nanotecnologias (INESC MN), Lisbon, Portugal

<sup>2</sup>IPFN, Instituto Superior Técnico, Universidade de Lisboa, Portugal

<sup>3</sup>i3N, Departamento de Física, Universidade de Aveiro, 3810-193 Aveiro, Portugal

<sup>4</sup>Departamento de Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, Madrid, Spain

<sup>5</sup>INL - International Iberian Nanotechnology Laboratory, Braga, Portugal

\*Corresponding Author: [danielapereira@ctn.tecnico.ulisboa.pt](mailto:danielapereira@ctn.tecnico.ulisboa.pt)

Molybdenum oxide (MoO<sub>3</sub>) is a two dimensional (2D) wide band gap semiconductor that has been attracting attention for multiple applications such as biosensors, gas sensors, solar cells and lithium ion batteries. Its thermodynamically stable phase at room temperature, namely the orthorhombic phase ( $\alpha$ -MoO<sub>3</sub>), is composed by layers that are bonded in the [010] direction by Van der Waals forces, making it a material that is easily exfoliated into thin layers with high surface/volume ratio. Furthermore, by varying the concentration of oxygen vacancies it is possible to change, in a controlled way, the intrinsic insulating behaviour of MoO<sub>3</sub> to a semiconductor or even metallic behaviour. This is indeed observed in the MoO<sub>x</sub> ( $3 \geq x > 2$ ) and MoO<sub>2</sub> phases, respectively.[1,2]

In this work,  $\alpha$ -MoO<sub>3</sub> thin exfoliated crystals and pseudo-layers are obtained by a mechanical exfoliation process using adhesive tape and by the Pulsed Laser Ablation in Liquid technique, respectively. These materials are incorporated into field effect transistor (FETs) using two different processing strategies. Both FET devices show a modulation of the channel resistance with gate bias. A decrease of channel resistance with increasing gate voltage is observed, which agrees with the characteristic n-type behavior of  $\alpha$ -MoO<sub>3</sub>. Complementary, structural, morphological and optical characterization of MoO<sub>3</sub> pseudo-layers by Raman spectroscopy, Scanning Electron Microscopy, UV/Vis absorbance and X-ray diffraction will be discussed. As the  $\alpha$ -MoO<sub>3</sub> is intrinsically insulating, it is necessary to modify its electrical properties to work in a FET device. In this way, ion implantation will be presented as a technique to increase the conductivity of this material. Indeed, an increase of conductance of about four orders of magnitude is observed for higher oxygen fluences, which is attributed to the formation of extended defects and new suboxide minority phases.[3,4]

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# APPLICATION OF CARBON FIBRE-BASED ELECTRODES IN STRUCTURAL LITHIUM-ION BATTERIES

**Beatriz Arouca Maia<sup>1,2,3</sup>, Natália Magalhães<sup>1</sup>, Eunice Cunha<sup>1</sup>, Raquel Santos<sup>1,3</sup>, Nuno Correia<sup>1,3</sup>, Maria Helena Braga<sup>1,2,3</sup>**

<sup>1</sup>INEGI – Institute of Science and Innovation in Mechanical and Industrial Engineering, 4000-014 Porto, Portugal  
email: bmaia@inegi.up.pt

<sup>2</sup>DEF, FEUP – Engineering Physics Department of the Faculty of Engineering of University of Porto, 4200-465 Porto, Portugal

<sup>3</sup>LAETA – Associated Laboratory of Energy, Transports and Aeronautics, 4200-265 Porto, Portugal

Correspondence: mbraga@fe.up.pt

The importance of energy storage systems is reflected in our daily life, from wireless devices to power-grid technologies, especially in the transportation industry. The urgency in optimising the already established systems is pretty clear in our society; it is mandatory to reduce our carbon footprint by implementing new and innovative technologies, minimising the impact of our everyday activities. One step to achieve these goals is to, firstly, reduce the mass of the overall battery systems (fewer and lighter materials mean less waste). This could be perfectly accomplished in the 80s sci-fi movies by designing a flying drone where the outer pieces could be all made of batteries. This concept is not much science fiction anymore. Structural materials are, more than ever, proof of how science and technology can evolve to optimise materials' traits. In this work are reported the preliminary results of the development of the structural electrodes to apply, as the ultimate goal, in a lithium-ion structural battery. Structural batteries are all-solid-state devices where the possibility to reduce the overall system mass is followed by good electrochemical and mechanical properties. [1] Some approaches are reported in the literature with several architectural designs; in this case, the final gadget is constituted by doped carbon-fibre electrodes with a solid polymer electrolyte. Lithium iron phosphate ( $\text{LiFePO}_4$ ) is one of the most used standard cathode materials due to its features of low cost, relatively good theoretical capacity ( $170 \text{ mAh.g}^{-1}$ ), favourable reversibility, environmentally friendliness, high chemical, electrochemical and thermal stability and good operating potential ( $3.4 \text{ V vs Li/Li}^+$ ). [2] Notwithstanding, some problems arise concerning ionic and electrical conductivity. Additionally, poor interface properties are achieved in the commercial solutions.

In this work, approaches have been made to turn LFP into a greener cathode by changing the usual NMP solvent and tuning its properties to increase both ionic and electrical conductivity. Additionally, its coating was made not in the typical carbon-doped aluminium foil but instead in a carbon-fibre reinforced polymer (CFRP) sheet. By doping its interface, efforts in using CFRP as anodes were also made. Coin and pouch cells were produced and analysed first against lithium metal and then against the produced anodes. Electrochemical, mechanical and chemical analyses were performed and discussed. A laminated structure made of carbon fibres with a polymeric electrolyte will be the final result of the present study.

## Acknowledgements

BAM, NM, EC and RS thank the “FLY.PT—Mobilize the Portuguese aviation industry to disrupt the future urban air transport” project, co-financed by the European Regional Development Fund (ERDF) through Portugal 2020. M.H.B. thanks the CAVALI project, with reference POCI-01-0247-FEDER-047728, co-funded by the ERDF through COMPETE 2020 under the PORTUGAL 2020 Partnership Agreement and FCT UIDP/50022/2020 EMERGING TECHNOLOGIES—LAETA.

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# Evidence of a Cluster Spin-Glass Phase in the Skyrmion-Hosting GaMo<sub>4</sub>S<sub>8</sub> compound

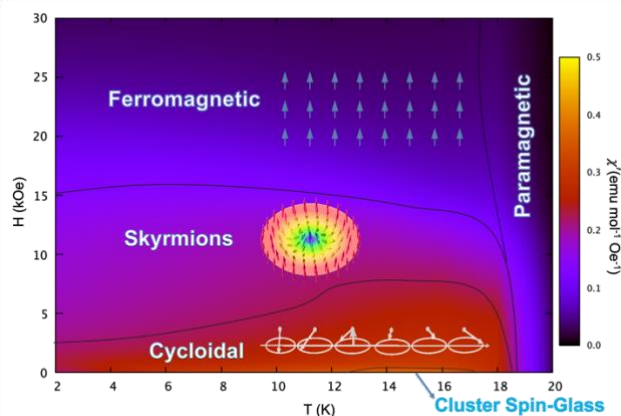
José F. Malta,<sup>1,2</sup> Marta S. C. Henriques<sup>1</sup>, José A. Paixão<sup>1</sup>, António P. Gonçalves<sup>2</sup>

<sup>1</sup> CFisUC, Department of Physics, University of Coimbra, Portugal

email: jap@uc.pt

<sup>2</sup> C2TN, Department of Nuclear Science and Engineering, Instituto Superior Técnico, Portugal

GaMo<sub>4</sub>S<sub>8</sub> is a poorly known lacunar spinel where skyrmions have only been reported very recently [1]. It belongs to the  $AM_4X_8$  family, where  $A$  is a post-transition metal,  $M$  is a transition metal and  $X$  is a chalcogenide, whose most celebrated member is GaV<sub>4</sub>S<sub>8</sub>, a compound where the existence of skyrmions has been firmly established [2]. In this work, we obtained pure amounts of polycrystalline GaMo<sub>4</sub>S<sub>8</sub> through a new synthetic route, a solid-state reaction between MoS<sub>2</sub> and Ga, at high temperature (1000 °C). Composition and purity were confirmed through the Rietveld refinement of the powder XRD pattern, where no additional phases were found. The magnetic phase diagram was investigated using DC (VSM) and AC magnetometry, affording novel insights into the physical properties of GaMo<sub>4</sub>S<sub>8</sub>. In addition to the skyrmionic phase present below  $T_C$  for applied magnetic fields between 5 kOe and 15 kOe, we have found evidence for the presence of a cluster spin-glass phase ( $T_g=15.3$  K), observed under small applied magnetic fields. An additional anomaly at 5 K, detected in AC susceptibility measurements, correlates with an anomalous behaviour of the magnetic field dependence of the specific heat at low temperature. Figure 1 shows the magnetic phase diagram obtained from our measurements for GaMo<sub>4</sub>S<sub>8</sub> [3].



**Figure 1** – Magnetic Phase Diagram for GaMo<sub>4</sub>S<sub>8</sub> obtained from AC Susceptibility Measurements.

## Acknowledgements

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# Reentrant spin-glass and magnetic skyrmions in the $\beta$ -Mn-type alloy $\text{Co}_7\text{Zn}_7\text{Mn}_6$

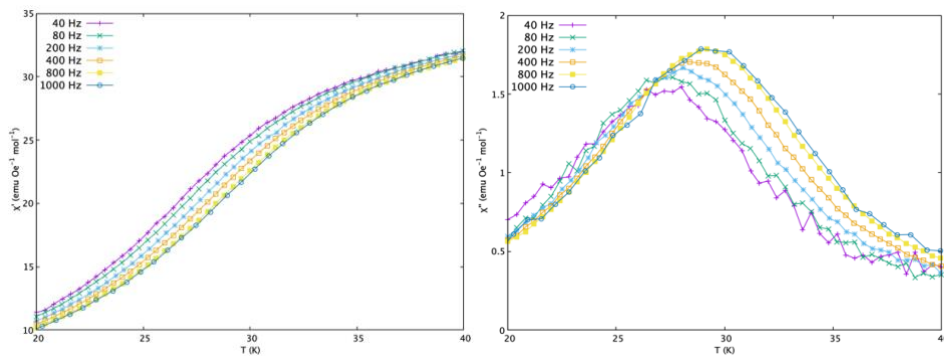
José F. Malta<sup>1,2</sup>, Marta S. C. Henriques<sup>1</sup>, José A. Paixão<sup>1</sup>, António P. Gonçalves<sup>2</sup>

<sup>1</sup> CFisUC, Department of Physics, University of Coimbra, Portugal

email: jap@uc.pt

<sup>2</sup> C2TN, Department of Nuclear Science and Engineering, Instituto Superior Técnico, Portugal

$\beta$ -Mn-type alloys based on  $\text{Co}_x\text{Zn}_y\text{Mn}_z$  stoichiometry ( $x+y+z=20$ ) are a family of cubic chiral magnets that crystallise into  $P4_132/P4_332$  space groups, known for hosting magnetic skyrmions. Skyrmions are swirling spin structures carrying a topological quantum number that occurs due to the competition between the ferromagnetic exchange and the Dzyaloshinskii-Moriya interaction. They were first observed in MnSi and later in a few magnetic compounds belonging to other cubic non-centrosymmetric space groups.  $\text{Co}_8\text{Zn}_8\text{Mn}_4$ , e.g., can host near room-temperature skyrmions and, as such, is considered as one of the most promising skyrmionic compounds for applications [1]. Neutron-scattering studies on  $\text{Co}_7\text{Zn}_7\text{Mn}_6$  have found evidence for disordered skyrmions near a reentrant spin-glass transition  $T_g$  ( $\sim 30$  K), as well as a region of ordered skyrmions below  $T_C$  ( $\sim 160$  K) [2]. In this work, we will present a detailed study on the  $\text{Co}_7\text{Zn}_7\text{Mn}_6$   $\beta$ -Mn-type alloy, focused on the low temperature spin-glass behaviour and on the skyrmionic phase observed below  $T_C$ . The synthesised sample was characterised by XRD and EDS and magnetisation studies performed *via* VSM and AC Susceptibility to map the phase diagram and characterised in detail the re-entrant spin-glass transition.



**Figure 1** – Low-temperature AC susceptibility (left:  $\chi'$  ; right:  $\chi''$  ) in the spin-glass phase of  $\text{Co}_7\text{Zn}_7\text{Mn}_6$ , showing a large frequency shift of the dissipative (imaginary) component typical of a spin-glass state.

## Acknowledgements

J.F. Malta PhD grant is supported by FCT- Fundação para a Ciência e a Tecnologia through ChemMat PhD programme. Access to TAIL-UC facility supported by the QREN-Mais Centro programme ICT\_2009\_02\_012\_1890 is gratefully acknowledged. This work was partially supported by funds from FEDER (Programa Operacional Factores de Competitividade COMPETE) and from FCT under the projects UIDB/FIS/04564/2020, UIDP/FIS/04564/2020 and PTDC/FIS-MAC/32229/2017.

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# AQUISIÇÃO E TRATAMENTO DE DADOS EXPERIMENTAIS COM A CALCULADORA GRÁFICA

**J. Jorge Teixeira<sup>1</sup>, Ana M. Dias<sup>2</sup>**

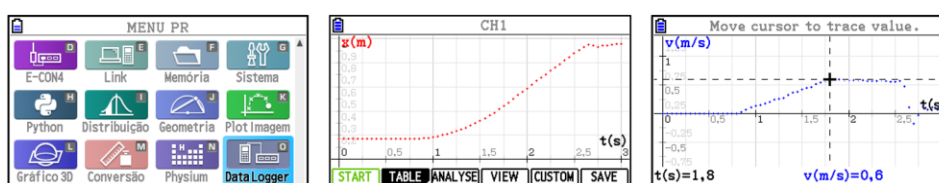
<sup>1</sup> Agrupamento de Escolas Dr. Júlio Martins, Av. 5 de outubro, 5400-017 Chaves, Portugal.

email: jjsteixeira@gmail.com

<sup>2</sup> Casio School Coordinator, Rua do Polo Sul, n.º 2 4.ªA, 1990-273 Lisboa, Portugal.

Cada vez mais alunos e professores de Física e Química A recorrem à calculadora gráfica (CG) em atividades que requerem o traçado de gráficos e de retas de ajuste aos dados experimentais. Os exames nacionais de Física e Química A incluem questões cuja resolução requer o recurso a uma CG. Assim, a CG é uma tecnologia que o aluno, no ensino secundário, tem de ter disponível e a única a que pode aceder nos exames. Para a aquisição e tratamento de dados experimentais, professores e alunos utilizam, normalmente, diverso *software* e *hardware*, sendo necessário algum tempo de familiarização. Quanto maior for o número de programas e instrumentos utilizados, menos tempo os alunos têm disponível para outras tarefas como, por exemplo, previsão de resultados, tratamento de dados, comunicação de resultados, discussão de resultados, etc. Deste modo, somos de opinião que a utilização da CG pelos alunos, em conjunto com uma aplicação específica, é uma mais-valia no processo ensino/aprendizagem ao nível da rentabilização do tempo, dos custos e da utilização de metodologias ativas. Para o efeito, foi criada, em 2021, a aplicação *Data Logger* para as calculadoras CASIO [1].

Assim, este trabalho tem como principais objetivos mostrar as potencialidades da aplicação *Data Logger*, indicar alguns exemplos de atividades (figura 1) e apresentar um manual para o professor com sugestões, montagem do material, procedimento para a recolha de dados com a calculadora e o tratamento de dados recolhidos nas atividades laboratoriais de Física dos 10.º e 11.º anos. A realização das atividades laboratoriais com a aplicação referida foi implementada numa turma do 10.º ano, constituída por 18 alunos. Verificou-se que a utilização simultânea da CG e da aplicação *Data Logger* foi um fator de motivação para os alunos, o número de ensaios realizados pelos alunos duplicou, todos os alunos partilharam os resultados com a turma e houve uma melhoria de 19% nas questões dos testes relacionadas com as atividades laboratoriais, em relação às atividades laboratoriais de química onde não utilizaram a CG.



**Figura 1.** Alguns ecrãs da calculadora obtidos numa atividade experimental.

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# OVERVIEW OF TODAY'S BATTERY ENERGY STORAGE SYSTEMS AND TECHNOLOGIES FOR GRID ENERGY SOLUTIONS

**Hesham Khalifa<sup>1,2,\*</sup> and Maria Helena Braga<sup>1,3,\*</sup>**

<sup>1</sup>Engineering Physics Department, Faculty of Engineering, University of Porto (FEUP), 4200-465 Porto, Portugal.

<sup>2</sup>Department of Physics, Faculty of Science, Damanhour University, Postal code 22514 Damanhur, Beheira Governorate, Egypt.

<sup>3</sup>LAETA-INEGI, Engineering Physics Department, FEUP, University of Porto, 4200-465 Porto, Portugal

\*Correspondence: [hesham@fe.up.pt](mailto:hesham@fe.up.pt) (H.K.); [mbraga@fe.up.pt](mailto:mbraga@fe.up.pt) (M.H.B.)

**Keywords:** renewable energy sources; battery energy storage system (BESS); uninterruptible power supply (UPS); stakeholders; datacenters; job roles.

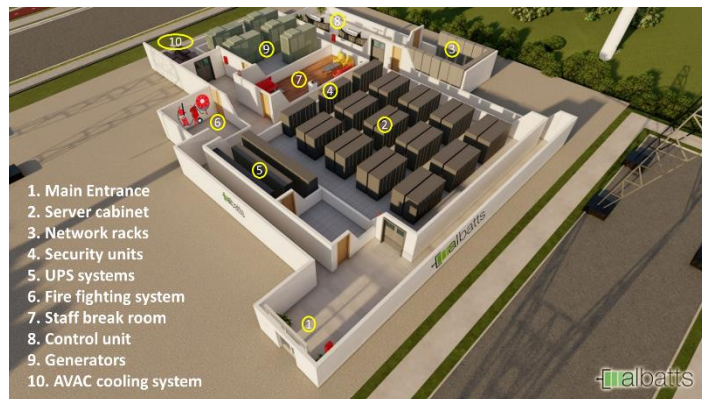
The environmental pollution and the depletion of mineral resources have encouraged the world to move into renewable energy sources for electricity generation. The EU has been lowering its reliance on coal to meet its climate goals of carbon neutrality by 2050 and a 55% reduction in emissions by 2030.

The penetration of renewable energy into the grid has recently increased, thanks to advancements in digital technologies like artificial intelligence, blockchain, and predictive analytics, notably since the cost of using renewable energy sources in electricity generation has been significantly reduced. However, renewable energy sources exhibit unexpected electricity outputs that degrade the grid's stability and durability. One of the practical solutions to guarantee an uninterrupted supply of power under all conditions is integrating a battery energy storage system (BESS) into the grid. A BESS is a multi-component energy storage system that stores varying amounts of electrochemical energy and uses it later for various purposes, such as data centers. BESS is the heart of renewable energy research, closing the gap to a fully green-powered society with no adverse consequences. Figure 1 illustrates a design of a green datacenter based on a battery energy storage system (BESS). The advances in battery technology make BESS a light and affordable solution for residential and commercial use, including smart homes, large-scale industrial facilities, and utility grids.

In this overview, we will discuss these and other key drivers that have transformed the global energy storage market in recent years, as well as the challenges that must be overcome. We will also spotlight the uninterruptible power supply (UPS), battery energy storage technologies, stakeholders, datacenters, and job roles and skills.

## Acknowledgments

This work was supported by the Alliance for Batteries, Training and Skills ALBATTs project, with reference 612675-EPP-1-2019-1-SE-EPPKA2-SSA-B, Funded by the Erasmus<sup>+</sup> Sector Skills Alliances Programme.



**Figure 1** Layout for designed ALBATTs datacenter integrated with battery energy storage system (BESS)

# SCANNING KELVIN PROBE - CHARACTERIZATION OF SOLID-STATE DEVICES

A. N. Guerreiro<sup>1</sup> and M. Helena Braga<sup>2\*</sup>

<sup>1</sup>Engineering Physics Department, FEUP, University of Porto, 4200-465 Porto, Portugal;  
nguerreiro@fe.up.pt

<sup>2</sup>LAETA-INEGI, Engineering Physics Department, FEUP, University of Porto, 4200-465 Porto, Portugal;

\*Correspondence: mbraga@fe.up.pt;

The socio-economic development of contemporary societies is due to the great technological development of energy production and distribution. This development was at the expense of the consumption of fossil fuels with environmental consequences. The environmental problems created by the use of fossil fuels, force us to rethink the entire paradigm of energy production. Since the beginning of the 21<sup>st</sup> century, we have had a significant investment in the production of electricity from alternative energies. An energy transition is needed to enable sustainable development and a stable electricity supply. In addition to this, we have had a high and fast technological development from mobile phones to biotechnology.

Concerning that, devices like cells and batteries can contribute to that main objective by grouping knowledge from various areas of physics, materials science, electrochemistry, digital technology, and engineering. The study of new materials that can improve and innovate the performance of cells/batteries that are capable and reliable to face the new energy challenges is extremely important. The study of materials for electrodes, and electrolytes, namely, ferroelectric and thermoelectric properties can be translated into a significant advance[1][2]. In that regard, the study of different materials with the Scanning Kelvin Probe (SKP) technique can improve a better understanding of the surface phenomena between different materials like conductors' metals (copper, aluminum, and zinc), dielectrics (oxides), and shell materials like cork. These studies were complemented with Electrochemical Impedance Spectroscopy (EIS) and Cyclic Voltammetry (CV) studies to characterize the electrochemistry of the pair of metals with electrolyte disjoined by an oxide. These studies can guide the choice of material groups for more efficient battery cells.

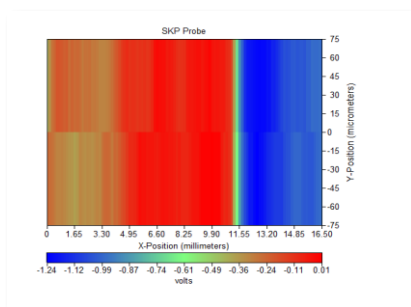


Figure 1. Gradient of the electrical potential of the Cu\_ZnO\_Al obtained by SKP

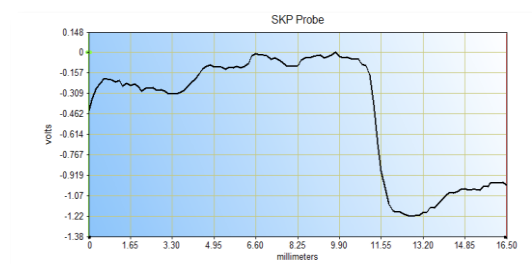


Figure 2. Evolution of the electrical potential of the Cu\_ZnO\_Al obtained by SKP

**Keywords:** Scanning Kelvin Probe; ferroelectric electrolytes; energy storage; electrical conductivity; ionic conductivity; materials science

## References

- [1] M. H. Braga, A. J. Murchison, J. B. Goodenough, Data in Brief, 29 (2020) 105339.
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## Organização

### COMISSÕES da FÍSICA 2022

Comissão Organizadora Local	Comissão Organizadora Encontro
<ul style="list-style-type: none"><li>• André Pereira (FCUP)</li><li>• Célia Sousa (FCUP)</li><li>• Joaquim Agostinho (FCUP)</li><li>• Eduardo Castro (FCUP)</li><li>• Maria de Fátima Mota (FCUP)</li><li>• Ana Rita Lopes Mota</li><li>• M<sup>a</sup> Deolinda Campos (DESPF/AEAS)</li></ul>	<ul style="list-style-type: none"><li>• M<sup>a</sup> Deolinda Campos (DESPF/AEAS)</li><li>• Ana Rita Lopes Mota</li><li>• José María Pastor Benavides (Presidente de la DEDF)</li><li>• Carmen Carreras Béjar. (Vicepresidenta de la DEDF)</li><li>• Luis Afonso (SPF/AE Benfica)</li></ul>
Comissão Científica Conferência	Comissão Científica Encontro
<ul style="list-style-type: none"><li>• Joana Espain (FEUP)</li><li>• Luís Manuel Fernandes Rebouta (UM)</li><li>• Pedro Teles (FCUP),</li><li>• Ana Rita Lopes Mota</li></ul>	<ul style="list-style-type: none"><li>• Miguel Angel Queiruga Dios. (UBurgos)</li><li>• Maria Fernanda Miguélez Pose (UACoruña)</li></ul>

- 
- Bernardo G. Almeida (UM)
  - Célia Sousa (FCUP),
  - Deolinda Campos (AEAS),
  - Eduardo V. Castro (FCUP),
  - Francisco Marinho (UTAD),
  - Fernando Amaro (UC),
  - Joaquim Agostinho Moreira (FCUP),
  - José Almeida (UTAD)
  - Maria de Fátima de Mota (FCUP)
  - Nuno Araújo (FCUL)
  - João A. Santos (UTAD)
  - José Pires Marques (SPFDSI/DFFCUL)
  - M<sup>a</sup> Carmo Lopes (IPOCoimbra)
  - Constança Providencia (UC/DFN)
  - Katharina Lorenz (INESCmn)
  - Sofia Andringa (LIPLx)
  - Ricardo Gonçalo (DFUC/LIPC)
  - Nuno Castro (LIPUM)
  - Gonçalo Figueira (ISTUL)
  - Manuel Marques (DFA/FCUP)
  - Carlos Silva (IPFN)

- 
- Luis Matias (DEGGEUL)
  - Paulo Relvas (UALG)
  - Augusto Fitas (DFUEvora)
  - João Pedro Araujo (DFA/FCUP)

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### **Secretariado e Comunicação**

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- Isabel Alves
  - Maria José Couceiro
-





## Apoios e Patrocínios

### Institucional



## Ouro



### MTBrandão

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A M.T. Brandão, constituída em 1984, atua num setor de elevada tecnologia, tendo como principais clientes as indústrias petrolíferas, alimentares e químicas, entre outras empresas industriais e tecnológicas, bem como instituições de ensino e investigação científica.

É uma empresa que se caracteriza pela experiência, especialização e qualificação e completa linha de produtos e soluções. A M.T. Brandão desenvolve a sua atividade nas seguintes Áreas de Negócio: Instrumentos de Análise de Laboratório e Processo, Caracterização de Materiais, Lasers e Optoelectrónica, Imagem, Teste e Medida, Didática e Assistência e Serviços.



### EQS

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Prestador de serviços global, a EQS atua no domínio da Gestão de Ativos Críticos ao longo de todo o seu Ciclo de Vida, desenvolvendo serviços de Ensaios, Inspeção, Certificação, Monitorização, Consultoria, Formação e Outsourcing. Trabalhando no sentido de superar constantemente as expectativas dos seus clientes, a sua especialização técnica, soluções e tecnologia inovadoras visam aumentar os níveis de segurança, integridade e desempenho das operações. Realiza consultoria técnica e de Terceira Parte procurando evitar a ocorrência de acidentes graves, otimizar a produção, reduzir custos de manutenção e garantir a conformidade.



SISTEMAS DE ENSINO E PESQUISA PARA LABORATORIO  
EXpT

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### EXPT – Sistemas de ensino e pesquisa para laboratório

EXPT tem como objetivo a comercialização de equipamento para investigação, material didático, científico e de laboratório, numa perspetiva de prestação de serviços. Este posicionamento leva a empresa a oferecer um conjunto abrangente de soluções assentes numa política de produtos e serviços da mais elevada qualidade e rigor.

A gama de produtos comercializados pela empresa baseia-se em equipamentos fabricados pelas nossas representadas, Phywe (Alemã), Gampt (Alemã), Gunt (Alemã), Peaktech (Alemã), Niryo (Frância) e Spectrumtechniques (EUA), Tytorobotics (EUA)

Os clientes da EXPT são Universidades, Institutos Politécnicos, Centros de Formação do IEFP, Escolas Profissionais, Escolas Secundárias com ensino profissionalizante do Ministério da Educação.

## Prata



### HBK Fibersensing

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**HBK FiberSensing, S.A.**, é uma unidade de negócios da HBK, situada na Maia, dedicada ao desenvolvimento e produção de sistemas avançados de monitorização baseados na tecnologia de Fiber Bragg Grating (FBG).

Originalmente fundada em 2004 e adquirida em 2014 pela Hottinger Baldwin Messtechnik (HBM), a empresa gere hoje todas as actividades ópticas da HBK, incluindo o desenvolvimento de produtos, fabrico e desenvolvimento de negócios, enquanto trabalha em conjunto com a organização global de vendas, que marca actualmente a sua presença em mais de 80 países em todo o mundo.

Suportada por competências que vão desde a tecnologia de fibras óticas à optoelectrónica, electrónica digital e instrumentação, a empresa comercializa um vasto portefólio de sensores óticos, interrogadores e aplicações de software, bem como soluções de monitorização personalizadas de acordo com os requisitos específicos do cliente, tornando-a num parceiro preferencial para acordos OEM.

## Regular



### TMG Automotive

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O TMG Group baseia-se em 80 anos de história empresarial definida pela inovação orientada para o valor. O segredo do nosso sucesso são as relações e os fortes laços que tecemos com os nossos parceiros.

Exportando para mais de 40 mercados e gerindo uma vasta carteira de negócios - indústria têxtil e automóvel, retalho, vinificação, energia hidroelétrica - estamos empenhados na qualidade e no crescimento sustentável enraizados na visão do nosso fundador.

Na vanguarda da qualidade e da tecnologia, orgulhamo-nos de ser uma das principais empresas têxteis. Esforçamo-nos por minimizar a pegada ambiental das nossas operações e queremos ter um impacto positivo no planeta. No centro de tudo o que fazemos estão as pessoas, uma equipa com um espírito de vanguarda que encara o futuro com a confiança e o entusiasmo experientes daqueles que têm uma visão clara. A força do nosso sonho é tão forte como sempre.



### inanoEnergy

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A InanoEnergy desenvolve e fornece soluções inovadoras para a Internet das Coisas (IOT) e a recolha de energia, utilizando micro e geradores termoelétricos, triboelétricos e piezoelétricos flexíveis e de alta eficiência adaptados às necessidades das empresas privadas, e criando tecnologia inovadora que proporciona grandes vantagens à indústria nacional. Também prestamos serviços de consultoria (incluindo investigação e desenvolvimento) para grandes empresas nacionais e internacionais que procuram aplicações específicas e feitas à medida.



### INESCTEC

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INESC TEC - Instituto de Engenharia de Sistemas e Computadores, Tecnologia e Ciência

O INESC TEC é um Laboratório Associado multidisciplinar de orientação internacional com mais de 35 anos de experiência em I&D e transferência de tecnologia.

A missão do INESC TEC é promover avanços científicos e tecnológicos, assim como inovação de base tecnológica, através da transferência de novos conhecimentos e tecnologias para a indústria, serviços e administração pública.

O INESC TEC junta academia, empresas, administração pública e sociedade, aplicando o conhecimento e os resultados gerados na investigação em projetos de transferência de tecnologia, procurando criar valor e uma relevância social imediata.

Com 6 polos no Porto (sede), Braga e Vila Real, o INESC TEC agrega 13 Centros de I&D, estruturados em quatro domínios temáticos - Informática, Engenharia Industrial e de Sistemas, Redes de Sistemas Inteligentes, e Energia.

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