Book of Abstracts

3rd Condensed Matter Physics National Conference

28th February-2nd March, 2022

Faculdade de Ciências, Universidade de Lisboa

3rd CMPNC LISBOA 2022
3rd Condensed Matter Physics National Conference

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CONTENTS

GENERAL INFORMATION

The 3rd Condensed Matter Physics National Conference is organized by the Condensed Matter Physics Division of the Portuguese Physical Society, and held in Lisboa, 28th February – 2nd March, 2022.

The venue is at Faculdade de Ciências, Universidade de Lisboa, Campo Grande, 1749-016 Lisboa.

Buiding C6, room 6.1.36.

The main objective of the meeting is to promote contacts between scientists working in Condensed Matter Physics, to share experiences, to spread the latest information on progress in their specialties and related fields, to gain visibility for their research, to put young researchers interacting with their peers and seniors, and to develop professionally. The Condensed Matter Physics Division aims also at create a space for discussion and reflection of the area in Portugal and its international impact.

The program includes invited talks, oral and poster communications.

Proceedings are published in the EPJ Web of Conferences journal.

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PROGRAMA

1st day -28th February		
9:00	**Reception** **Posting of session A posters**	9:00
10:00	**Opening session**	10:00
10:15	**Session 1: Low-Dimensionality and Quantum Systems** *Chairman: Eduardo Castro*	10:15
10:15	**Invited** **Aires Ferreira** **"Spin-orbit coupling phenomena in two-dimensional layered materials"**	10:15
11:00	**Coffee Break / Posters (session A)**	11:00
11:30	**Session 2: Phase Transitions and Critical Phenomena:** *Chairman: João Amaral*	11:30
11:30	**Invited** **V. Konotop** **"Steering of light in photonic Moiré lattices"**	11:30
12:15	Oral 1: Henrique Prates, "Coherent oscillations and self-trapping of BECs in shallow supperlattices"	12:15
12:30	Oral 2: Diogo Pinto, "The cell adaptation time sets a minimum length scale for patterned substrates"	12:30
12:45	Oral 3: Danilo Silva, "Effect of droplet deformability on shear thinning in a 3D channel"	12:45
13:00	**Lunch**	13:00
14:15	**Announcements**	14:15
14:30	**Session 3: Semiconductors and Dielectrics** *Chairman: Mikhail Vasilevskiy*	14:30
14:30	**Invited** **Rui Vilão** **"Muons as local probes in semiconductors and dielectrics"**	14:30
15:15	Oral 1: Bruna Silva, "Dielectric Properties of Ruddlesden-Popper Ca3Mn2O7 thin films prepared by Pulsed Laser Deposition"	15:15
15:30	Oral 2: Mariana Gomes, "Phase sequence and properties of piezoelectric $K_{0.5}Na_{0.5}NbO_3$ ceramics sintered by different routes"	15:30
15:45	Oral 3: Vanda Pereira, "Topological insulator/ferromagnetic insulator heterostructures: Bi_2Te_3 on magnetite and iron garnets	15:45
16:00	**Coffee Break / Posters (session A)**	16:00
16:30	**Session 4: - Strongly Correlated Electron Systems** *Chairman: Joaquín Rossier*	16:30
16:30	**Invited** **P.Sacramento** **"Correlations and dynamic phase transitions in topological systems"**	16:30
17:15	Oral 1: Bruno Murta, "Gutzwiller Wave Function on a Quantum Computer"	17:15
17:30	Oral 2: Carolina Marques, "The surface of Sr_2RuO_4: from unconventional orders to a magnetic-field tuned van Hove singularity"	17:30
17:45	Oral 2: Gonçalo Catarina, "Hubbard parent model for Haldane spin-1 chains"	17:45
18-20	**Posters (session A)**	18-20

2nd day – 1st March		
9:00	**Removing session A posters and posting of session B posters**	9:00
9:30	**Session 5: Nanotechnology and Devices** *Chairwoman: Susana Freitas*	9:30
9:30	**Invited** **Ricardo Ferreira** **"Magnetic nano-devices applied to disruptive solutions for sensing, communications and information processing"**	9:30
10:15	Oral 1: Sofia Teixeira, "Optimised topological insulators towards magnetoelectric spin-orbit meso logic devices"	10:15
10:30	Oral 2: Catarina Dias, "Bio/electronic interfaces for neuroprostetics"	10:30
10:45	Oral 3: Joaquim Leitão, "Role of defects on the electrical performance of Cu(In,Ga)Se_2 based solar cells: experimental and theoretical study	10:45
11:00	**Coffee Break / Posters (session B)**	11:00
11:30	**Session 6: Soft Matter and Biophysics** *Chairman: Nuno Araújo*	11:30
11:30	**Invited** **M. Alves** **"Purely elastic flow instabilities of complex fluids"**	11:30
12:15	Oral 1: Pedro Patrício, "Convection patterns gradients of non-living and living micro-entities in hydrogels"	12:15
12:30	Oral 2: Cristovão Dias, "How to design cell-mediated self-assembled colloidal scaffolds"	12:30
12:45	Oral 3: Rodrigo Coelho, "Director alignment at active nematic-isotropic interfaces"	12:45
13:00	**Lunch**	13:00
14:15	**Divisão: Quantum Matter @ PT**	14:15
14:30	**Session 7: Low-Dimensionality and Quantum Systems** *Chairman: Ricardo Dias*	14:30
14:30	**Invited** **Joaquín Rossier** **"Magnetic 2D crystals: magnons and interlayer coupling"**	14:30
15:15	Oral 1: Miguel Gonçalves, Hidden dualities in 1D quasiperiodic lattice models	15:15
15:30	Oral 2: David Perkins, "Anomalous Weak Localisation Phase in Ultra-Clean van der Waals Heterostructures"	15:30
15:45	Oral 3: Lucas Sá, "Random Matrix Theory of Open Quantum Systems"	15:45
16:00	**«Coffee Break / Posters (session B)**	16:00
16:30	**Session 8: Low-Dimensionality and Quantum Systems** *Chairman: João V. Lopes*	16:30
16:30	**Invited** **Nuno Peres** **"Metallic gratings covered with 2D materials: a route to polaritonics"**	16:30
17:15	Oral 1: João Pires, "Band Spectrum Deformation due to Small Clusters of Atomic-Sized Impurities in Dirac-Weyl Semimetals"	17:15
17:30	Oral 2: Hugo Terças, "Topological plasmons in graphene field-effect transistors with odd viscosity"	17:30
17:45	Oral 3: Diogo Cunha, "Optical Kerr effect in graphene under pulsed illumination in the visible spectral range"	17:45
18-20	**Posters (session B)**	18-20

3rd day – 2nd March		
9:00	**Removing session B posters**	9:00
9:30	**Session 9: Magnetism** *Chairwoman: Laura Pereira*	9:30
9:30	**Invited** **G. Kakazei** **"Spin-wave spectroscopy of individual ferromagnetic nanoelements"**	9:30
10:15	Oral 1: Artem Bondarenko, “Detecting a shadow of the magnetic vortex core”	10:15
10:30	Oral 2: Rui Vilarinho da Silva, “Magnetic and vibrational non-critical anomalies in $RFeO_3$”	10:30
10:45	Oral 3: Rafael Vieira, “High-throughput ab-initio calculations for magnetocaloric materials”	10:45
11:00	**Coffee Break**	11:00
11:30	**Session 10: Functional Materials** *Chairman: José A. Paixão*	11:30
11:30	**Invited** **M Mendes** **"The New Horizons of Photovoltaics improved with Light Management"**	11:30
12:15	Oral 1: João Belo da Silva, “Contraction and giant negative thermal expansion at the nanoscale in the $Gd_5(Si,Ge)_4$ multifunctional materials”	12:15
12:30	Oral 2: Samuel Santos, “Insights and correlations between EFG and spontaneous electric polarization in HIF materials”	12:30
12:45	**Closing session**	12:45

INVITED TALKS

I1 - SPIN-ORBIT COUPLING PHENOMENA IN TWO-DIMENSIONAL LAYERED MATERIALS

Aires Ferreira

Department of Physics, University of York

Spin-orbit coupling (SOC)—a relativistic interaction which entangles a particle's motion with its quantum mechanical spin—is fundamental to a wide range of physics phenomena, spanning from the formation of topological insulators to the spin Hall effect of light. Recent years have seen remarkable progress in probing, enhancing and tailoring SOC effects in atomically thin materials and their interfaces. From the electrical control of spin-valley coupling in bilayer graphene [1] to reversible spin-charge conversion in graphene on transition metal dichalcogenides at room temperature [2], these discoveries challenge our previous notions of the possible behaviour of spin-orbit coupled electrons at interfaces. In this talk, I will discuss recent proposals for probing and exploiting the rich interplay of spin and lattice-pseudospin spin degrees of freedom afforded by two-dimensional layered materials [3] and present our new findings [4].

References

[**1**] "*Anisotropic spin currents in graphene*", https://physics.aps.org/articles/v11/s108

[**2**] "*Optimal charge-to-spin conversion in graphene on transition-metal dichalcogenides*", M. Offidani, M. Milletarì, R. Raimondi, and A. Ferreira, Phys. Rev. Lett. 119 (2017); "*Gate-tunable reversible Rashba−Edelstein effect in a few-layer Graphene/2H-TaS2 heterostructure at room temperature*", L. Li, *et al*, ACS Nano 14 (2020); "*Proposal for unambiguous electrical detection of spin-charge conversion in lateral spin valves*", S. A. Cavill, C. Huang, M. Offidani, Y.-H. Lin, M. A. Cazalilla and A. Ferreira, Phys. Rev. Lett. 124 (2020)

[**3**] "*Skew-scattering-induced spin-orbit torque at 2D material/ferromagnet interfaces*", F. Sousa, G. Tatara and A. Ferreira, Phys. Rev. Res. 2 (2020); "Effect of proximity-induced spin-orbit coupling in graphene mesoscopic billiards", A. Barbosa, J. Ramos, and A. Ferreira, Phys. Rev. B 103 (2021)

[**4**] "*Twist-Angle-Controlled Spin Galvanic Effect in 2D Heterostructures*", A. Veneri *et al*. in preparation (2022).

I2 - STEERING OF LIGHT IN PHOTONIC MOIRÉ LATTICES

Vladimir V. Konotop

Centro de Física Teórica e Computacional and Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, Portugal

Nowadays, moiré structures attract increasing attention across different areas of physics. Light propagation through moiré patterns created in photorefractive photonic crystals is one of them. The great tunability of parameters of photorefractive crystals allows for exploring a wealth of geometries and potential landscapes of monolayered moiré patterns in the linear and nonlinear regimes. In this talk, I will review recent experimental and theoretical results on localization and delocalization of light in linear moiré lattices [1], on the effect of the twist angle on generation and stability of two-dimensional solitons [2], and on excitation of multifrequency solitons in quadratic media with resonantly interacting fundamental field and second harmonic [3]. Extensions of the presented results and perspectives will be briefly discussed.

References

[1] P. Wang, Y. L., Zheng, X. F. Chen, C. M. Huang, Y. V. Kartashov, L. Torner, V. V. Konotop, and F. W. Ye, Nature **577**, 42 (2020).

[2] Q. Fu, P. Wang, C. Huang, Y. V. Kartashov, L. Torner, V. V. Konotop, and F. Ye, Nat. Phot. **14**, 663 (2020).

[3] Y. V. Kartashov, F. Ye, V. V. Konotop, and L. Torner, Phys. Rev. Lett. **127**, 163902 (2021).

I3 - MUONS AS LOCAL PROBES IN SEMICONDUCTORS AND DIELECTRICS

Rui Vilão

CFisUC, Department of Physics, University of Coimbra, Coimbra, Portugal.

The use of positive muons as local probes has become a standard, albeit exotic, technique for obtaining microscopic information in condensed matter physics, materials science and chemistry, through the use of the set of muon spin rotation, relaxation and resonance techniques (μSR). Positive muons are mostly used as microscopic magnetometers, highly sensitive to local magnetic fields and hyperfine interactions. In non-magnetic semiconductor and dielectric systems, the behaviour of positive muons as light pseudo-isotopes of hydrogen has been successfully explored. A brief review of the use of positive muons for the modelling of the hydrogen impurity in semiconductors and dielectrics will be presented. The role of hydrogen as a compensating impurity, as an effective-mass shallow donor impurity or as a passivating impurity will be addressed. Additionally, recent developments on the use of low-energy muon beams to characterize semiconductor interfaces will be shown, including the microscopic description of an interface distorted layer attributed to the long-range strain caused by defects.

I4 - CORRELATIONS AND DYNAMIC PHASE TRANSITIONS IN TOPOLOGICAL SYSTEMS

Pedro Sacramento

Departamento de Fisica and CeFEMA, Instituto Superior Tecnico,

Av. Rovisco Pais , 1049-001 Lisboa, Portugal

The time dependence of interacting topological systems in non-equilibrium states, that result from different kinds of perturbations, is considered.

A characterization of topological phases in terms of quasilocal operators (topological correlators) is discussed, as well as their time evolution.

As a result of sudden quenches, dynamical quantum phase transitions are considered using the Loschmidt rate, the topological correlators and Green's functions. Under the effect of a unitary evolution, topological invariants remain unchanged but physical quantities (such as the Hall conductance) signal changes in topology. We have considered a photoinduced topological transition, resonantly targeting topological many-body states with pulses.

I5 - MAGNETIC NANO-DEVICES APPLIED TO DISRUPTIVE SOLUTIONS FOR SENSING, COMMUNICATIONS AND INFORMATION PROCESSING

Ricardo Ferreira

INL | International Iberian Nanotechnology Laboratory,

Avenida Mestre José Veiga, 4715-330 Braga, Portugal

Magnetic Tunnel Junctions are complex devices with rich physical mechanisms that are being widely used in a large spectrum of applications. Historically, the push for these devices was fuelled by magnetic hard disk drives that required increasingly sensitive devices to be able to read increasingly smaller magnetic fields from increasingly smaller magnetic bits. But nowadays, these extremely sensitive sensors are being used in new ways and areas of application. The example of industrial tool monitoring and predictive maintenance of heavy industrial equipment will be presented to illustrate the advantages of this type of sensors with respect to more conventional solutions.

When the devices dimensions are reduced to the range of ~50-600nm, the spin transfer torque mechanism comes into play and with it the ability to explore the dynamic interaction between electrical currents and micromagnetic magnetization configurations. Vortex nano-oscillators will be presented as an example of devices that explore this type of interactions. Departures from the ideal vortex model and real devices will also be show as well as the impact of the real-device effects on applications such as wireless communications and neuromorphic computation.

Finally, the versatile nature of the devices, together with its multi-functional nature (the very same device can perform very different tasks when integrated in a system) will be demonstrated with examples of truly multi-functional devices that integrate in the same pillar more than one function as well as small “spintronic circuits” targeting neuromorphic computation.

I6 - PURELY ELASTIC FLOW INSTABILITIES OF COMPLEX FLUIDS

Manuel A. Alves

Departmento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto,
Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

Viscoelastic fluids are common in our daily life and are also important in different industrial applications. Due to their nonlinear rheology, viscoelastic fluid flows often lead to complex and counterintuitive behaviour and, above critical conditions, drive the onset of instabilities even under creeping flow conditions.

We present an overview of different types of purely elastic flow instabilities and how they can be simulated numerically. The governing equations and the techniques used to enhance numerical stability are briefly described [1]. Illustrative numerical results and current challenges related with the high Weissenberg number problem are discussed, with emphasis on the use of the rheoTool open source library [2,3].

References

[1] M.A. Alves, P.J. Oliveira, F.T. Pinho (2021). Numerical methods for viscoelastic fluid flows, *Annual Review of Fluid Mechanics*, Vol. 53: 509-541.

[2] F. Pimenta, M.A. Alves (2017). Stabilization of an open-source finite-volume solver for viscoelastic fluid flows, *Journal of non-Newtonian Fluid Mechanics*, Vol. 239: 85-104.

[3] https://github.com/fppimenta/rheoTool

I7 -MAGNETIC 2D CRYSTALS: MAGNONS AND INTERLAYER COUPLING

Joaquín Rossier

INL - International Iberian Nanotechnology Laboratory,
Avenida Mestre José Veiga, 4715-330 Braga, Portugal

In this talk I will cover 3 topics. First, I will provide an overview [1] of the nascent field of magnetic 2D crystals and their heterostructures, known as Van der Waals heterostructures.

Second, I will discuss the crucial role played by magnons in 2D materials, how can magnons be probed in inelastic spectroscopy [2], the concept of topological magnons [3] and how to compute magnons starting from first principles calculations [3,4]. Third, I will discuss a new type of interlayer exchange [5], based on hybridization, that can lead to very large proximity effect in heterostructures that combine magnetic 2D layers, such as CrI3, and graphene.

[1] Magnetic Two-Dimensional Chromium Trihalides: A Theoretical Perspective
D. Soriano, M. I. Katsnelson, and J. Fernández-Rossier, Nano Letters 20, 9, 6225–6234 (2020)

[2] Probing magnetism in 2D van der Waals crystalline insulators via electron tunnelling
Dahlia R. Klein, David MacNeill, Jose L. Lado, David Soriano, Efrén Navarro-Moratalla, Kenji Watanabe, Takashi Taniguchi, Soham Manni, Paul Canfield, J. Fernández- Rossier, Pablo Jarillo-Herrero, Science 360, 1218 (2018)

[3] Topological Magnons in CrI3 monolayers: an itinerant fermion description
A. Costa, D. Santos, N. M. R. Peres, J. Fernández-Rossier, 2D Materials 7 045031 (2020)

[4] Nonreciprocal magnons in a two-dimensional crystal with out-of-plane magnetization
Marcio Costa, N. M. R. Peres, J. Fernández-Rossier, A. T. Costa, Physical Review B **102,** 014450 (2020)

[5] Electrically tunable hybridization magnetic-proximity effect.
C. Cardoso et al., in preparation

Funding from FCT PTDX/FIS-MAC/2045/2021 is acknowledged.

I8 - METALLIC GRATINGS COVERED WITH 2D MATERIALS: A ROUTE TO POLARITONICS

Nuno Peres

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International Iberian Nanotechnology Laboratory (INL), 4715-330 Braga, Portugal

Metallic diffraction gratings have been intensively studied for more than a century. Its theoretical study started with the work of A. Sommerfeld back to 1899. The interest in metallic gratings was kept alive for many decades to follow with the work of U. Fano and A.Maradudin extensively contributing to its understanding. The latter author contributed with a number of works to the understanding of metallic gratings taking roughness into account. By the 1980's, gratings were considered understood and the topic faded away. Coming from a completely different area of physics, the discovery of 2D materials around 2004-2005 gave rise to a new field of research in nanophotonics based on these new types of systems. In particular scientists regain interest in gratings when these are covered with 2D materials. This new type of system supports new types of polaritons whose study is still in its infancy. In this communication we will present an ongoing theoretical study of a metallic grating covered with two types of 2D materials, an insulator and a conductor. We will see the emergence of new types of polaritons with far reaching consequences in applications to sensing and nanophotonics.

I9 - SPIN-WAVE SPECTROSCOPY OF INDIVIDUAL FERROMAGNETIC NANOELEMENTS

G.N. Kakazei[1], S.A. Bunyaev[1], K.Y. Guslienko[2,3], M. Huth[4], A.V. Chumak[5], O.V. Dobrovolskiy[5]

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[5] Nanomagnetism and Magnonics, Faculty of Physics, University of Vienna, 1090 Vienna, Austria

Focused electron beam induced deposition (FEBID) is a technique of choice for direct-writing of nano-architectures with applications in nanomagnetism, magnon spintronics, and superconducting electronics. Here, a series of our recent experiments on direct-write FEBID nanomagnets and their use in nanomagnonics will be discussed. First, an original spatially resolved approach for spin-wave spectroscopy of individual circular magnetic elements with sample volumes down to about 10^{-3} μm^3 will be presented [1]. The key component of the setup is a coplanar waveguide whose microsized central part is placed over a movable substrate with well-separated CoFe-FEBID nanodisks which exhibit standing spin-wave resonances. The circular symmetry of the disks allows for the deduction of the saturation magnetization and the exchange stiffness of the material using an analytical theory. Next, using this approach, the engineering of the magnetic properties of CoFe-based nanodisks fabricated by FEBID will be demonstrated [2]. The material composition in the nanodisks was tuned *in situ* via the e-beam waiting time in the FEBID process and their post-growth irradiation with Ga ions. The achieved saturation magnetization M_s variation in the broad range from 720 to 1430 emu/cm^3 continuously bridges the gap between the values of widely used magnonic materials such as Permalloy and CoFeB. Further, nanovolcanoes - nanodisks overlaid by nanorings – will be introduced as purpose-engineered 3D architectures for nanomagnonics [3]. The extension of 2D nanodisks into the third dimension allows for engineering their lowest eigenfrequency with 30% smaller footprints. The nanovolcanoes can be viewed as multi-mode microwave resonators and 3D building blocks for nanomagnonics. Finally, spin-wave phase shifters upon a single nanogroove milled by a focused ion beam in a Co–Fe microsized magnonic waveguide, characterized by all-electrical spin-wave spectroscopy, will be described [4]. By varying the groove depth and the in-plane bias magnetic field, we continuously tune the spin-wave phase and experimentally evidence a complete phase inversion. The proposed phase shifter can easily be on-chip integrated with spin-wave logic gates and other magnonic devices.

References

[1] Dobrovolskiy, O.V. et al. (2020), Spin-wave spectroscopy of individual ferromagnetic nanodisks. Nanoscale, 12, 21207-21217.
[2] Bunyaev, S.A. et al. (2021). Engineered magnetization and exchange stiffness in direct-write Co–Fe nanoelements. Appl. Phys. Lett., 118, 022408.
[3] Dobrovolskiy, O.V. et al. (2021). Spin-wave eigenmodes in direct-write 3D nanovolcanoes. Appl. Phys. Lett., 118, 132405.
[4] Dobrovolskiy, O.V. et al. (2019). Spin-wave phase inverter upon a single nanodefect. ACS Appl. Mater. Interfaces, 11, 17654-17662.

I10 -THE NEW HORIZONS OF PHOTOVOLTAICS IMPROVED WITH LIGHT MANAGEMENT

M. J. Mendes, H. Aguas, E. Fortunato, R. Martins

CENIMAT|i3N, Department of Materials Science, School of Science and Technology, NOVA University of Lisbon and CEMOP/UNINOVA, Campus de Caparica, 2829-516 Caparica, Portugal

Photovoltaic (PV) technology is currently in an embryonic stage, since there is still a long way to trailblaze to reach an optimized exploitation of the immense solar power available on Earth. Here we will cover some of the most exciting developments that are being cooked in lab, but will find industrial application in a near future.

The first challenge of solar electricity is concerned with efficiency. For that, recent breakthroughs have been attained with the multi-band PV concept realized with perovskite solar cells impregnated with colloidal quantum dot arrays, which can potentially reach 50% solar-to-electricity efficiency with single-junction devices, thereby surpassing the traditional *Shockley-Queisser* limits.

The second challenge is cost-effectiveness. To tackle that, photonic structures with dimensions comparable to the sunlight wavelengths are now regarded as the preferential solutions to enhance the power/cost ratio of thin photovoltaic devices via light trapping. For instance, we have designed photonic thin-film cell architectures capable of efficiency improvements up to 100% with respect to planar reference solar cells!

The third main challenge of solar electricity has to do with Storage. In that respect, artificial photosynthesis is one of the best ways to protect the environment while producing carbon-based fuels, because it closes the anthropogenic carbon cycle. We will present Photovoltaic-Electrochemical (PV-EC) integrated systems, enhanced via light management (photonic) strategies, capable of converting sunlight and CO_2 into usable carbon-based fuels with high efficiency.

ORAL COMMUNICATIONS

O1 - COHERENT OSCILLATIONS AND SELF TRAPPING OF BECS IN SHALLOW SUPPERLATTICES

Henrique C. Prates[1,*], Dmitri A. Zezyulin[2], Vladimir V. Konotop[1]

[1]Centro de Física Teórica e Computacional and Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal.

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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 self-trapping, coupled solitons, etc. We show that an alternative, and in several aspects even more general, setting allowing the physical realization of the mentioned phenomena is a BEC loaded in either quasiperiodic lattices or in superlattices emulating almost periodic functions on a finite spatial interval. Such lattices even being sufficiently shallow allow efficient localization of spatially separated BECs even in the linear regime, for multiple low-energy levels below the mobility edge. In this work, we analyze the dynamics of two and four coupled BEC clouds in the presence of attractive and repulsive interatomic interactions. The reduced discrete models governing the system are a dimer and quadrimer. A full-scale study of the meanfield dynamics is performed numerically within the framework of Gross-Pitaevskii equation, which reveals the conditions for the localization as well as the limits of a few-mode approximation.

Acknowledgements

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O2 - THE CELL ADAPTATION TIME SETS A MINIMUM LENGTH SCALE FOR PATTERNED SUBSTRATES

Diogo E. P. Pinto[1,2], Gonca Erdemci-Tardogan[3,4], M. Lisa Manning[3], Nuno A. M. Araújo[1,2]

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The emergence of spatial patterns of cells is critical for morphogenesis, collective cell motion, and wound healing. A strategy to generate these patterns in vitro, which is already being investigated by several experimental groups to generate organoids or organs-on-chip, uses patterned cultured substrates to regulate the space-dependent properties of the tissue. But, the impact of external stimuli in the cell morphology and mechanics requires a hierarchy of biochemical processes that sets a finite adaptation time scale which can extend over hours. We show that the fidelity of patterns depends on the relation between the diffusion (τ_D) and adaptation (τ) times of the cells. Numerical results for the self-propelled Voronoi model reveal that the fidelity decreases with τ/τ_D, a result that is reproduced by a continuum reaction-diffusion model. The competition between these two-time scales translates into a minimum length scale for the patterns, with several practical implications [1].

Figure 1. Schematic representation of the system. We consider a confluent tissue on a squared substrate with two regions of equal linear length, which differ in the target value of the shape index ($P_0/\sqrt{A_0}$) of cells. Where P_0 and A_0 are the cells preferred perimeter and area respectively.

Acknowledgements

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O3 - EFFECT OF DROPLET DEFORMABILITY ON SHEAR THINNING IN A 3D CHANNEL

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The collective behaviour of fluid emulsions often emerges from the properties of individual microscopic droplets that compose it. In confined microenvironments, where the size of the droplet is comparable to the width of the channel, droplet deformability has an impact on the macroscopic flow properties [1]. We study deformable droplets suspended in a fluid flowing through a 3D channel with neutral wetting (Fig. 1). We find a discontinuous shear thinning transition, which depends on the droplet deformability [2]. The capillary number is the main parameter that controls the transition. We also notice significant differences in the velocity profiles when compared with 2D studies in the literature [3]. Due to the 3D structure, the surrounding fluid flows through the droplets. To obtain these results, we improved and extended to 3D a multicomponent Lattice Boltzmann method which prevents the coalescence between the droplets.

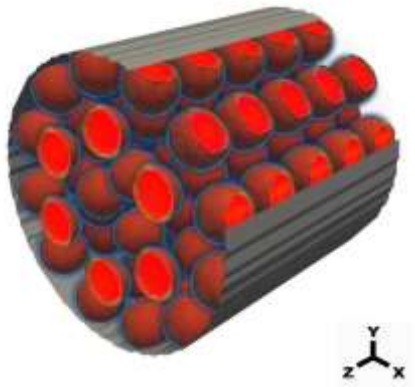

Figure 1. 105 droplets non-close packed in a 3D cylindrical channel. An external force in the z-direction drives the flow.

4

Acknowledgements

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O4 - DIELECTRIC PROPERTIES OF RUDDLESDEN–POPPER $Ca_3Mn_2O_7$ THIN FILMS PREPARED BY PULSED LASER DEPOSITION

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Naturally Layered Perovskite structures with improper ferroelectricity [1, 2], such as the Ruddlesden-Popper calcium manganite compound $Ca_3Mn_2O_7$, offer an alternative route to achieve non-expensive and high-performance room temperature multiferroic magnetoelectricity for information storage, sensors, and actuators or low power energy-efficient electronics. They allow exploring oxygen octahedra nonpolar rotations and cation site displacement to attain non-centrosymmetry. Additionally, 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. However, the preparation conditions to obtain the $Ca_3Mn_2O_7$ phase with the Ruddlesden-Popper structure need to be optimized and their properties have not yet been explored.

As such, thin films of $Ca_3Mn_2O_7$ have been prepared over $SrTiO_3$ substrates by Pulsed Laser Ablation, using a $Ca_3Mn_2O_7$ target. Polycrystalline $Ca_3Mn_2O_7$ was synthesized using a conventional high-temperature ceramic route. The structural studies show that in the films prepared on $SrTiO_3$, at 730 ºC, with 4 J/cm^2 laser fluence, 10^{-3} mbar oxygen pressure and with a postannealing process, the $Ca_2Mn_3O_7$ phase is stabilized, as confirmed by XRD and Raman Spectroscopy. The corresponding EDS analysis further gives a Ca/Mn atomic ratio of ~1.5:1, consistent with the presence of this phase. The magnetic properties were measured using a SQUID magnetometer, showing an antiferromagnetic transition at 110 K. The dielectric properties of the films show a relaxor-type behaviour (fig. 1), described by the Vogel-Fulcher-Tammann equation. The dielectric properties of the films will be discussed and presented, highlighting the phase evolution and stabilization in the films.

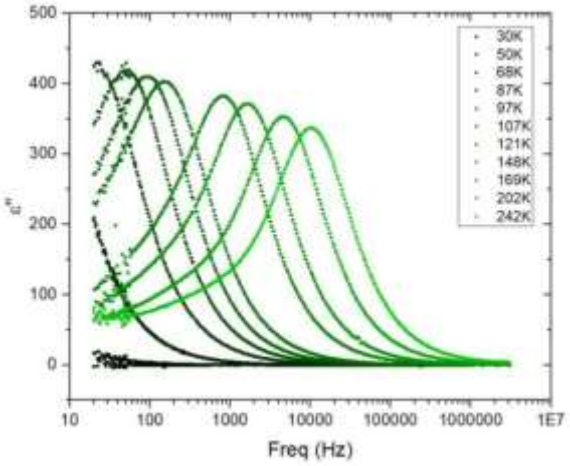

Figure 1. Imaginary permittivity in function of frequency for $Ca_3Mn_2O_7$.

Acknowledgements:

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O5 - PHASE SEQUENCE AND PROPERTIES OF PIEZOELECTRIC $K_{0.5}Na_{0.5}NbO_3$ CERAMICS SINTERED BY DIFFERENT ROUTES

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In order to substitute lead zirconate-titanate (PZT) based materials, due to its poisonous nature, some promising piezoelectric and friendly environment compounds are attracting growing attention, namely KxNa(1-x)NbO3 [1]. For the case of x=0.5, K0.5Na0.5NbO3 (KNN), the hightemperature cubic symmetry changes to a non-symmetric ferroelectric tetragonal structure at T3=700 K, becoming orthorhombic at T2=465 K, and finally stabilizing in a rhombohedral symmetry below T1=135 K [2]. Recently, theoretical calculations have predicted piezoelectric response enhancement when T3 become closer to T2 [3], in which sintering conditions could play an important role [4,5].

In this work, we revisit the phase transition sequence and the effect of the sintering process on the structure, lattice dynamics, and dielectric/polar properties of KNN ceramics prepared by conventional sintering, spark plasma sintering, and spark plasma texturing. From a comparative analysis of the overall experimental obtained results, we have observed that the phase transition sequence includes an unreported structural and polar phase at low temperatures, independently on the processing method. Moreover, apparent changes of the stability temperature interval of the different phases have been ascertained. The dielectric strength and the emergence of a dielectric relaxation phenomenon are also noticeably dependent on the processing method, which can be understood as an effect of the different grain size. The results here reported clearly point out towards the possibility to change physical properties following different sintering routes to improve device performance.

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O6 - TOPOLOGICAL INSULATOR/FERROMAGNETIC INSULATOR HETEROSTRUCTURES: Bi_2Te_3 ON MAGNETITE AND IRON GARNETS

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Breaking the time-reversal symmetry of a topological insulator (TI) can lead to interesting phenomena such as the quantum anomalous Hall effect. This can be experimentally achieved using the magnetic proximity effect in TI/ferromagnetic insulator (FI) heterostructures to magnetize the topological surface state at the interface.

Here, we report the growth and characterization of Bi_2Te_3 thin films on Fe_3O_4 (001), Fe_3O_4 (111), $Y_3Fe_5O_{12}$ (111) and $Tm_3Fe_5O_{12}$ (111) [1-3]. The growth by molecular beam epitaxy allows the formation of chemically clean interfaces. The observed anomalous Hall effect and a suppression of the weak anti-localization in the magnetoresistance are in agreement with the opening of a gap in the topological surface states induced by the magnetic proximity effect. Nonetheless, x-ray circular magnetic dichroism was not observed on the Te $M_{4,5}$ edges, suggesting that the weak van der Waals bonding between the TI/FI yields a transferred magnetic exchange too small to be detected by this technique.

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O7 - GUTZWILLER WAVE FUNCTION ON A QUANTUM COMPUTER

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One of the most promising applications envisioned for quantum computers is the simulation of strongly correlated electrons, particularly in regimes where the understanding of their behavior has eluded analytical and conventional numerical methods. To this end, a number of quantum algorithms to find the exact ground state of quantum many-body systems have been proposed [1-3]. In all cases, their success rests upon the ability to prepare an appropriate trial state, in the sense that it permits a mapping to the ground state in a reasonable number of steps. This requirement becomes more stringent the greater the system size due to the orthogonality catastrophe [4], in general, and to the concentration of distinctive features of the cost function landscape in exponentially small regions around minima [5], in the specific case of hybrid variational methods. Initializing an educated guess of the exact ground state is therefore important to make it possible to use quantum computers to explore quantum many-body phenomena that are inaccessible with traditional theoretical and computational methods.

Within this context, we have developed a routine [6] to prepare on a digital quantum computer the Gutzwiller Wave Function (GWF) [7]. This is a conceptually simple, physically-motivated ansatz that can be applied to the wide class of lattice models of correlated electrons where the electron-electron Coulomb repulsion is described, to leading order, in terms of the on-site Hubbard interaction. The GWF is a many-body state that captures some correlations between the electrons, thus overlapping more with the exact ground state than the noninteracting or mean-field ground states typically used as the starting point of quantum simulation algorithms.

In this talk, the routine to initialize the GWF on quantum hardware will be detailed, explaining, in particular, how to overcome the non-unitary form of the Gutzwiller projection. The scaling of this method, its concrete implementation in near-term gate-based quantum computers, and its integration in general quantum simulation algorithms will also be discussed.

Acknowledgements

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O8 - THE SURFACE OF Sr_2RuO_4: FROM UNCONVENTIONAL ORDERS TO A MAGNETIC-FIELD TUNED VAN HOVE SINGULARITY

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The nature of the enigmatic superconducting state in Sr_2RuO_4 remains an open question. Multiple experiments now indicate that it is closely linked to a van Hove singularity (vHs) in the vicinity of its Fermi level (E_F), however resolving what the order parameter (OP) is remains a challenge. Quasi-particle interference (QPI) imaging can in principle provide phase-sensitive information about the superconducting OP, however, tiny structural distortions in the surface layer seem to suppress superconductivity, resulting in a significant reconstruction of the Fermi surface and low energy electronic states [1]. Here, we use ultra-low temperature Scanning tunnelling microscopy to establish the existence of four vHs within 5 mV of E_F, unveiling a checkerboard charge order and hitherto unreported nematicity of the electronic states [1]. Including these orders into a tight-binding model, we can fully account for the four vHs. Continuum local density of states calculations which take into account the tunneling matrix elements show excellent agreement with the observed QPI patterns [2], Fig.1. We demonstrate that in magnetic fields up to 14 T, the vHs splits, and extrapolate that one of its branches reaches E_F at ~32 T – providing a text-book example of tuning towards a magnetic field-driven Lifshitz transition.

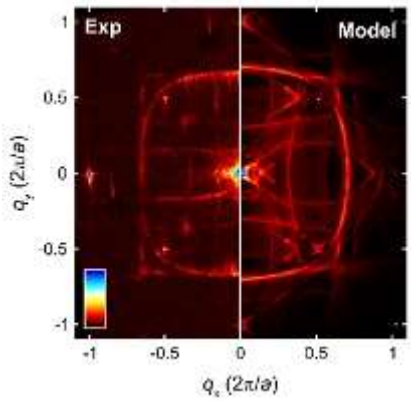

Figure 1. Comparison between an experimental quasiparticle interference measurement (left) with the Fourier transform of the calculated continuum local density of states image (right).

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O9 - HUBBARD PARENT MODEL FOR HALDANE SPIN-1 CHAINS

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The Haldane phase for chains of antiferromagnetically coupled $S = 1$ spins is one of the most celebrated topological states of matter, featuring gapped excitations [1] and fractional edge states [2,3]. However, the scarcity of both one-dimensional systems and sufficiently isotropic $S = 1$ spins in nature hampers the experimental research. Here we answer positively to the question of whether it is possible to realize this phase with a Hubbard model at half-filling. We propose a lattice where each $S = 1$ spin is stored in a four-site cluster (Figure 1). Using both exact diagonalization and density matrix renormalization group we show the equivalence between the Hubbard model in the low-energy regime and the spin-1 Heisenberg Hamiltonian with additional biquadratic terms. Moreover, we find that the non-interacting limit of the fermionic model describes a topological insulator and we conjecture that it belongs to the same topological class as the Haldane phase. Our work suggests an alternative route to explore the Haldane physics, with possible realizations through quantum dot arrays [4], dopant atoms [5] or polycyclic aromatic hydrocarbons [6].

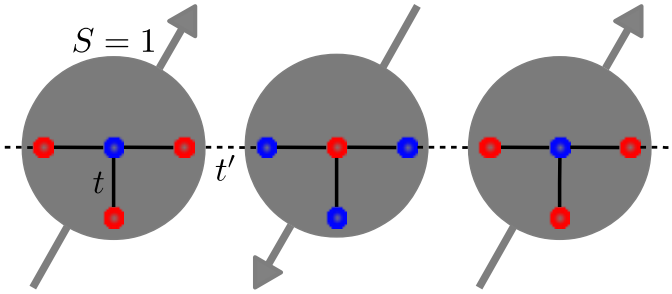

Figure 1. Four-site lattice as a realization of a spin-1 Haldane chain. Blue and red circles represent a fermionic lattice, with the hoppings t and t' indicated (colors denote the two sublattices). Hubbard model calculations at half-filling reveal that, for a wide range of parameters, i) each four-site cluster is a robust $S = 1$ spin object, ii) such $S = 1$ objects are coupled via an Heisenberg-like antiferromagnetic exchange. The emergent one-dimensional spin1 chain is in the Haldane phase, thus providing a realization of a quantum spin liquid.

Acknowledgements

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O10 - OPTIMISED TOPOLOGICAL INSULATORS TOWARDS MAGNETOELECTRIC SPIN-ORBIT MESO LOGIC DEVICES

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Spintronics has seen remarkable progress in the last decades. By combining well known concepts like Giant and Tunneling magnetoresistance with spin torques and control of domain walls, developments are foreseen in data storage [1] and logic, with new devices like the magnetoelectric spin-orbit MESO logic device [2]. New materials and nanostructures have also allowed several breakthroughs, from 2D materials to Topological Insulators.

Topological Insulators (TI) are a peculiar category of materials. Having been experimentally discovered only in 2007 [3], they have already shown great promise for a wide range of applications. Due to their performance in the control and switch of nanomagnets based on the Spin Orbit Torque (SOT), they could lead the advancements of new memory and logic devices.

One family of materials that has arisen within TIs is the Bi_2Se_3 family of semiconductors. They host a metallic state on their surface while having an insulating bulk. The metallic state is protected by time reversal symmetry and presents a spin texture. Moreover, due to their strong spin orbit coupling, high values of the Spin Hall angle θ_{SH} have been reported [4], leading to outstanding control of nanomagnets. Sb_2Te_3 is one of the members of this family, with the TI surface state being theorized in 2009 [5] and later observed [6]. However, it has not been widely studied due to its smaller band gap. Thus, it is not yet clear if it is a material of interest for SOT applications.

In this presentation, ion beam sputtered thin films of Sb_2Te_3 with thicknesses ranging from 35 to 200 nm are going to be explored. Their transport properties will be presented and discussed. By correlating the magnetoconductance and thermoelectric properties of the sputtered Sb_2Te_3 thin films, the exotic conduction of these materials will be untangled. Following the characterisation of these TI thin films, bilayers with magnetic permalloy thin films were produced and the current spin to charge conversion studies will be addressed. As the thin films have been made using a scalable inexpensive fabrication method, already employed in the industry, these results shine light into a novel topological insulator, with promising opportunities for future applications in spintronics.

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O11 - BIO/ELECTRONIC INTERFACES FOR NEUROPROSTETICS

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Significant efforts are being made to develop nanoscale electronic devices integrated into neuromorphic circuits capable of emulating the dynamics of natural synapses [1]. The coupling between neuronal populations via artificial synapses bears great potential for therapeutic strategies focused on the monitoring and control of neuronal electrical activity [2]. Such hybrid systems, effectively coupling biological and electrical components, are important milestones for the development of a new generation of neuroprosthetic devices aimed to address a number of challenging neurologic disorders. Memristors have gained attention as a core component is these hybrid systems, mainly because of their neuromorphic properties, small size and low power signature. Relevant proofs of concept have already been presented in the literature, but we argue that crucial aspects have not yet been demonstrated on how these memristor-based hybrid systems can effectively operate in a meaningful way [3]. Here we show, for the first time, how biological in vitro neuronal populations can be dynamically coupled with a memristive device acting as a synapstor, forming a hybrid bio-electronic system. We demonstrate that the conductance state of a memristor can be changed by the electrical activity of biological neurons and mediate a dynamic connection between isolated spiking neuronal populations. Our system connects biological neurons to microelectrodes, amplifier, memristor, stimulator, microelectrodes, and back to biological neurons, in an effective real-time configuration that does not use software nor simulations. Using our system, we can have neuronal population B being effectively activated if, and only if, there is a consistent firing pattern of activity in population A (network bursting activity). Importantly, we demonstrate that our artificial synapse is capable of short-term plasticity, dynamically changing its conductance level in both directions. Our results pave the way for further implementation of elements able to perform more complex modulatory operations in neuronal populations.

Acknowledgements

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O12 - ROLE OF DEFECTS ON THE ELECTRICAL PERFORMANCE OF $Cu(In,Ga)Se_2$ BASED SOLAR CELLS: EXPERIMENTAL AND THEORETICAL STUDY

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$Cu(In,Ga)Se_2$ (CIGS) based solar cells have the highest power conversion efficiency among cells based on thin film technology. This type of cells uses Cu poor films which implies the presence of a high defect density on the network. As a result, optical and electrical properties are strongly influenced by potential fluctuations in the material [1]. In this work, we study a set of three cells in which the Cu fraction was intentionally varied to modify the average depth of potential fluctuations. Photoluminescence, external quantum efficiency, and electrical measurements were performed. The bandgap energy and electrical parameters were evaluated for each sample and the average depth of fluctuations was discussed in the scope of theoretical models. Additionally, it was performed a theoretical study of the various types of fluctuations expected for CIGS, based on the analysis of extensions to the Shockley-Queisser model. The obtained results show that the cell performance is strongly affected by fluctuations, in particular, the loss observed in the open circuit voltage (V_{oc}) values. Among the various types of fluctuations (electrostatic, Urbach, and bandgap), the electrostatic ones have the dominant contribution to the V_{oc} losses [2]. Our results also show that potential fluctuations are important in the cell behavior at room temperature.

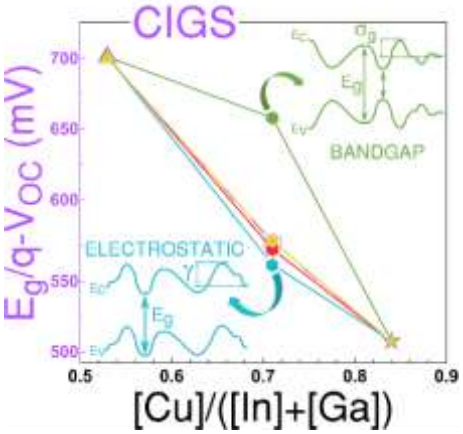

Figure 1. Experimental and calculated V_{OC} losses for samples with different [Cu]/([In]+[Ga]) values. Different types of fluctuating potentials were considered.

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O13 - CONVECTION PATTERNS GRADIENTS OF NON-LIVING AND LIVING MICRO-ENTITIES IN HYDROGELS

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Interfaces are vital in nature, where gradients of non-living and living entities build distinct yet continuous integrated living tissues. However, the common tissue fabrication methodologies often result in dissimilar interfaces, lacking continuity through the interfaced engineered tissues. Here, we induce thermal gradients in two injected fluid systems resulting in the temporal formation of mixing conductive streams. If preserved through sol-gel transition, this mechanism can be used to drive and pattern non-living and living entities in mixed hydrogels. In our presentation, we will focus on the physical mechanisms that drive convection, and present our numerical results, obtained from using Computational Fluid Dynamics methods. These results are then compared with the experimental part, showing the formation of convective lines which spatially drive microscale microparticle and cells when different temperatures are applied in the sequential injection of two gels.

Based on this finding, pure gellan gum (GG) and blended GG with methacrylated gelatin (GelMA) systems were used to program the formation of gradient features in hydrogels, such as microparticle and cells distribution patterns, polymeric bioactivity, degradation, controlled release, and stiffness.

Acknowledgements

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O14 - HOW TO DESIGN CELL-MEDIATED SELF-ASSEMBLED COLLOIDAL SCAFFOLDS

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A critical step in tissue engineering is the design and synthesis of 3D biocompatible matrices (scaffolds) to support and guide the proliferation of cells and tissue growth. Most existing techniques rely on the processing of scaffolds under controlled conditions and then implanting them *in vivo*, with questions related to biocompatibility and the implantation process that are still challenging. As an alternative, it was proposed to assemble the scaffolds *in loco* through the self-organization of colloidal particles mediated by cells. In this study, we combine experiments, particle-based simulations, and mean-field calculations to show that, in general, the size of the self-assembled scaffold scales with the cell-to-particle ratio. However, we found an optimal value of this ratio, for which the size of the scaffold is maximal when cell-cell adhesion is suppressed. These results suggest that the size and structure of the self-assembled scaffolds may be designed by tuning the adhesion between cells in the colloidal suspension [1,2,3].

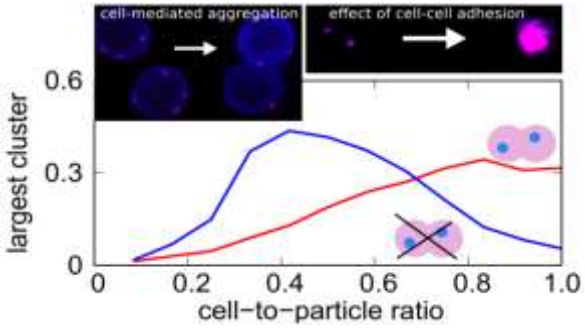

Figure 1. Simulation results for blocking and allowing cell-cell adhesion.

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O15 - ADVECTION-DIFFUSION OF ACTIVITY IN NEMATICS

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Efficient nutrient mixing is crucial for the survival of bacterial colonies and other living systems. This raises the question of whether the optimization of this feature through the bacterial motion was a factor in the evolution of bacterial shapes. In this work, we couple the hydrodynamic equations for active nematics with the advection-diffusion equation where the advected solute is the activity (representing the nutrients). In addition to molecular diffusion, the activity is transported by the flow and modifies it by means of the active stress. We find that the dispersion of activity is subdiffusive due to the movement of defects in both directions of the gradient. In addition, we found a non-monotonic behaviour of the subdiffusion coefficient as a function of the aligning parameter, which is related to the shape of the particles. Our simulations suggest that there is a shape that optimizes the dispersion of activity in active nematics.

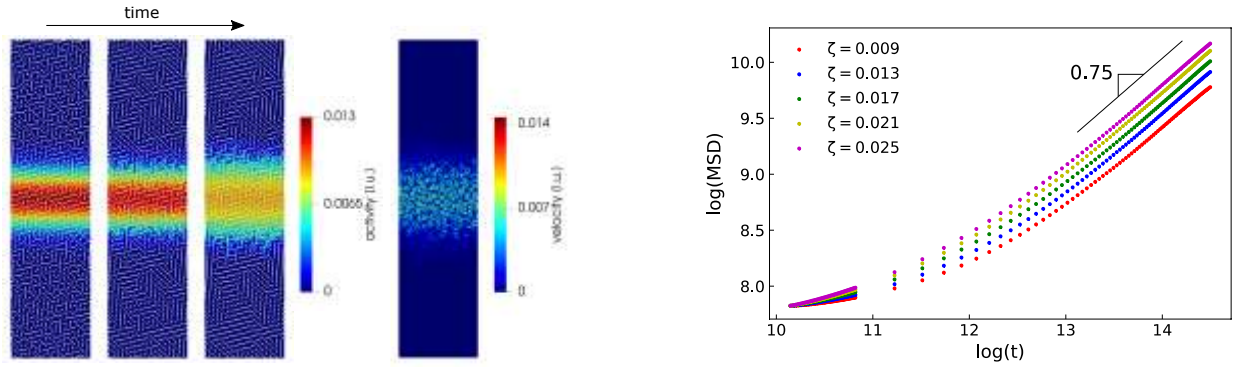

Figure 1. Dispersion of activity.

Acknowledgements

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O16 - HIDDEN DUALITIES IN 1D QUASIPERIODIC LATTICE MODELS

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Quasiperiodic systems (QPS) host a plethora of exotic properties ranging from localization to topological non-trivial states. Interest in quasiperiodic structures has been recently renewed due to their experimental relevance for describing optical and photonic lattices and the rise of Moiré systems.

The first steps to understanding quasiperiodic-induced localization steamed out of a celebrated 1D model, proposed by Aubry and André, that predicts a localization-delocalization transition arising simultaneously for all states in the spectrum [1]. This transition is a consequence of a special duality of the Aubry-André Hamiltonian. Later generalizations of this model give rise to single-particle mobility edges that may be highly non-trivial to determine and could only be analytically predicted in a few restricted fine-tuned models.

In this talk, we propose that the quasiperiodic-induced localization-delocalization transitions in generic 1D systems are associated with local hidden dualities that are generalizations of the Aubry-André case.

Based on this conjecture, we develop a method to compute mobility edges and duality transformations for generic QPS through their commensurate approximants. To illustrate the power of the method, mobility edges and duality transformations are obtained for a number of models, including generalized Aubry-André models [2-5] and coupled Moiré chains.

Our findings provide a useful and insightful way to study quasiperiodic-induced localization-delocalization transitions in 1D, including a working criterion for their emergence and for understanding the properties of eigenstates close to the transition.

Acknowledgements

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O17 - ANOMALOUS WEAK LOCALISATION PHASE IN ULTRA-CLEAN VAN DER WAALS HETEROSTRUCTURES

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Over the past two decades, two-dimensional (2D) van der Waals (vdW) materials have been the subject of numerous theoretical and experimental quantum transport investigations. In this talk we present a non-perturbative analysis of quantum corrections to the DC conductivity in 2D Dirac materials with symmetry-breaking spin-orbit coupling (SOC). We find that the commonly reported weak localisation to weak anti-localisation (WL-to-WAL) transition that is driven by increasing the strength of SOC is reversed in ultra-clean graphene heterostructures (i.e. WAL-to-WL). This counter-intuitive result can be traced back to the strong nonperturbative coupling between the pseudospin and spin degrees of freedom induced by SOC, which gaps out the delocalised modes of the Cooperon for large SOC strengths. Our results suggest that the nature of localisation in spin-orbit coupled 2D vdW materials is richer than first thought, highlighting the importance of non-perturbative methods in quantum interference studies of ultra-clean vdW heterostructures.

Acknowledgements

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O18 - RANDOM MATRIX THEORY OF OPEN QUANTUM SYSTEMS

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Describing complex interacting quantum systems is a daunting task. One very fruitful approach to this problem, developed for unitary dynamics, is to represent the Hamiltonian of a generic system by a large random matrix. This eventually led to the development of the field of quantum chaos. Here, we will discuss the recent application of (non-Hermitian) random matrix theory to open quantum systems, where dissipation and decoherence coexist with unitary dynamics. First, we consider the Lindblad generator of Markovian dissipation, for which a characteristic lemon-shaped spectrum has been identified in a variety of settings [1-3]. This allows us to characterize and constrain the timescales for relaxation and dissipation. Then, we focus on periodically driven open quantum systems and their discrete-time Kraus map representation [4]. We find a transition in the shape of the support of the spectrum of the Kraus map, occurring a critical value of the dissipation strength. The steady state, on the contrary, is not affected by the spectral transition, and its properties coincide with those of random Lindbladians, indicating universality. Finally, we briefly discuss how this work and its extensions [4,5] help in laying the foundations for systematic studies of generic open quantum systems. Of particular interest is the search for signatures of dissipative quantum chaos [5] and the study of more realistic local dissipative systems modeled as, e.g., quantum circuits [4].

Acknowledgements

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O19 - BAND SPECTRUM DEFORMATION DUE TO SMALL CLUSTERS OF ATOMIC-SIZED IMPURITIES IN DIRAC-WEYL SEMIMETALS

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The recent discovery of gapless three-dimensional semimetals turned Dirac-Weyl electrons into a hot topic [1] in condensed matter. The impact of disorder or impurities on Dirac-Weyl systems have attracted great interest [2], motivated by a putative quantum phase transition in which a semi-metallic phase (of vanishing density of states at the Fermi level) is destabilized into a diffusive metal phase. Recent studies based on continuum models [2,3] with dilute spherical wells/plateau indicate that delicate nodal boundstates hosted by (critical) impurities can actually destabilize the semi-metallic phase [3,4]. This transition happens in spite the fact that such configurations are fine-tuned and relies solely on a finite probability density for these to appear in the system. Meanwhile, independent studies [5] showed that there are no finite critical potential strengths for dilute d-impurities and nodal bound-states can only be formed via interference of two such nearby impurities. As these nodal modes are pivotal for the semimetal-to-metal transition, it becomes important to characterize how these emerge for a lattice impurity, as its structure grows more complex.

In this contribution, we show how critical impurities emerge from spherical clusters composed of equal atomic-sized scalar impurities in a lattice model. We employ the projected Green's function method [5], together with numerically evaluated clean green's function in position-space, to calculate the change in the (extensive) density of states and analyze how the structure of impurity resonances evolves with the cluster's radius. As this radius is decreased, one abridges the continuum prediction (a critical value inversely proportional to the radius [3]) with the diverging critical values expected for a single point-like impurity. Preliminary results are depicted in Figure 1.

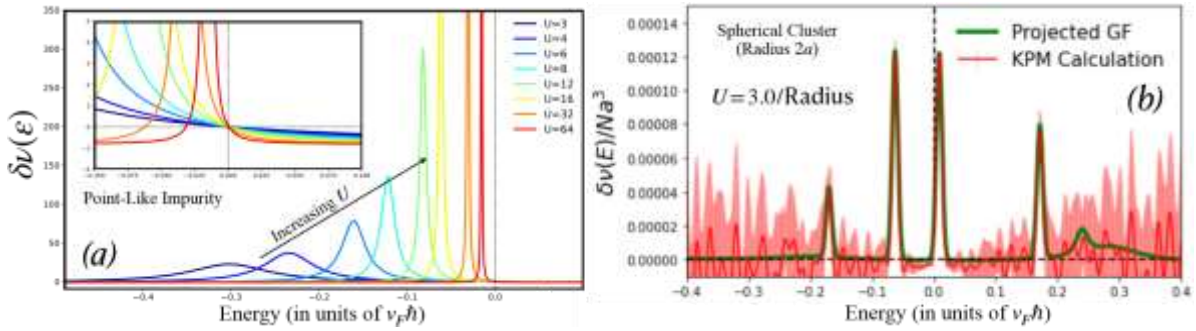

Figure 1. (a) Change in the DoS due to a single atomic-sized impurity of strength U. **(b)** Density of States' deformation due to a spherical cluster of radius 2a. Note that potential strength is slightly below the lowest critical value predicted by the continuum theory. Resonances above E=0 imply a deviation from this law. In red, the results are confirmed by more computationally expensive calculations using the kernel polynomial method.

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O20 - TOPOLOGICAL PLASMONS IN GRAPHENE FIELD-EFFECT TRANSISTORS WITH ODD VISCOSITY

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Graphene field-effect transistors (gFET) are appealing candidates for the next generation of TeraHertz (THZ) sources compatible with integrated-circuit. A prominent configuration is based on the Dyakonov-Shur (DS) instability, which is plausible in clean graphene channels operating in the hydrodynamic regime [1]. In the presence of magnetic fields, DS instabilities can be controlled by the cyclotron frequency, which sets the lower threshold for the spectral emission [2]. In this work, we exploit the high-magnetic field regime, in which collisions with phonons may lead to the appearance of odd (Hall) viscosity [3]. We show that topologically nontrivial plasmon modes can exist in gFETs. We further investigate how the topological phase - namely the lack of scattering to the bulk - may affect the stability criterion for the onset of DS instability

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O21 - OPTICAL KERR EFFECT IN GRAPHENE UNDER PULSED ILLUMINATION IN THE VISIBLE SPECTRAL RANGE

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Pump-probe spectroscopy is an experimental technique used to study ultrafast electrons' dynamics. A short pulse of a strong pump beam and, after a certain delay time, a weak probe beam are focused on the sample and the transmittance of the probe light is recorded. Owing to the strongly chirped nature of the probe pulse, by varying the delay times one can probe the system's response at different wavelengths. In the present work, this technique was applied to monolayer graphene deposited on a glass substrate, in the near infrared (central wavelength of the pump pulse λ=800 nm). The transmission of a second beam, the probe beam, with a large spectral width in the visible region, was altered by the presence of the pump via cross phase modulation. By comparing the signals measured with and without the pump pulse, differential transmittance spectra for graphene-covered and bare glass were recorded. The nonlinear response of graphene is larger than what has been measured previously for this 2D material, in the visible spectral range [1].

The theoretical part of this work is dedicated to the explanation of the experimental results obtained. During the short period of time (120 fs) when both pump and probe fields act on the system, the graphene's non-linear response (the optical Kerr effect) is described by the recently developed theory [2]. The pump beam also creates non-equilibrium electronic distributions of free electrons and holes, which relax towards lower energies through inelastic scattering processes on lattice phonons after the end of the pump pulse. This relaxation is studied using the Fokker-Planck equation for the non-equilibrium charge carriers' distribution, yielding a time-dependent linear optical conductivity seen by the probe beam. The real part of this conductivity is diminished by the state filling effect. The consideration of these two effects (Kerr and pump-induced transparency in graphene) allows us to explain the observed differential transparency spectra and to predict new effects to be observed in other excitation regimes.

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O22 - DETECTING A SHADOW OF THE MAGNETIC VORTEX CORE

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Over recent time magnetic vortices became the model magnetic soliton due to a number of simple to use analytical developments describing their behaviour, and the ease with which vortices are observed experimentally using common techniques. Traditionally, starting with the original Thiele work [1], vortices are treated in a running wave approximation, ignoring any deformations of its structure arising during the precession. Such theories are in excellent agreement with observed *kinetic* behaviour (although not without limitations), and they even find application for dynamics in finite-size geometries, e.g. Rigid Vortex Model [2].

In this talk we will explore a scenario in which vortices' magnetization is significantly deformed by a stray field of another magnetic vortex placed few nanometers above [3], such as seen on Fig. 1. This field is generated by small, out-of-plane core portion of the magnetic vortex, and is found to be strong enough to pull momenta out of plane in the coupled vortex. We observe the quasi-static behaviour of a mutually deformed magnetic vortex pair and compare it to that seen in micro-magnetic simulations.

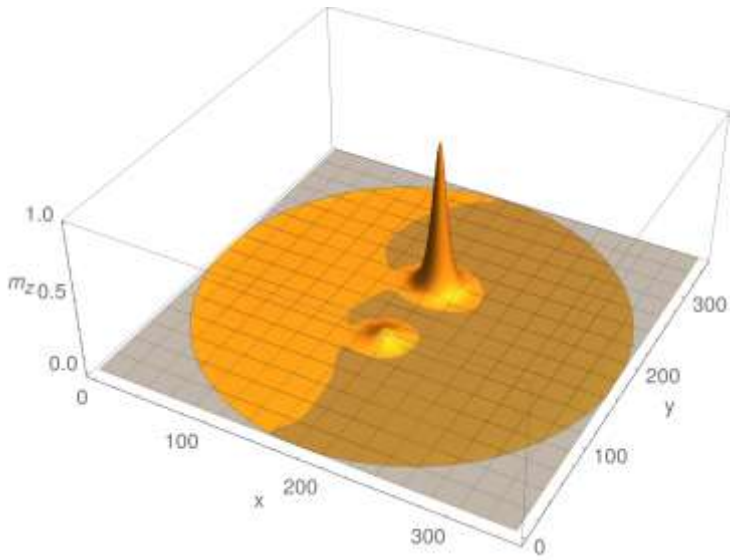

Figure 1. Planar cross-section of a simulated out-of-plane, m_z magnetization of a single vortex in a closely-stacked pair. A clearly defined "shadow" of a companion vortex is induced by the vortex core adjacent to it.

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O23 - MAGNETIC AND VIBRATIONAL NON-CRITICAL ANOMALIES IN $RFeO_3$

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Rare-earth orthoferrites ($RFeO_3$, R = rare-earth) have renewed the scientific interest due to their remarkable magnetic properties, spin-reorientation transitions and, more recently, by the discovery of ferroelectricity and multiferroicity in some of them [1]. The magnetic structure of $RFeO_3$ can be regarded as the superposition of interacting Fe^{3+} and R^{3+} spin sublattices. The Fe^{3+} spins strongly interact and order at much higher temperatures than the R^{3+} spins, that order antiferromagnetically only at low temperatures, usually below 10 K. At T_N between 623 and 740 K, the Fe^{3+} spin sublattice undergoes a magnetic phase transition into an $A_xF_yG_z$ canted antiferromagnetic Fe^{3+} spin structure. For R = Pr, Nd, Sm, Tb, Ho, Er, Tm, and Yb, there is also a spin-reorientation transition into the $C_xG_yF_z$ spin structure [1]. Between T_N and the temperature of R^{3+} spin ordering, the R^{3+} sublattice behaves paramagnetically, and can be polarized by the molecular magnetic field of the net ferromagnetic moment of the ordered Fe^{3+} sublattice. In the special cases with R = Nd, Sm, and Er, this ordering occurs in opposite direction of the Fe^{3+} sublattice, yielding a decrease of the total net magnetization that eventually vanishes at the compensation temperature, and reverses its sign below [2]. This behavior has been associated with the reinforcement of the R-R interactions. Despite the intensive research of the magnetic properties of these compounds, the origin of a set of anomalies observed in the M(T) curves, not ascribed to any magnetic phase transitions, have not been the subject of discussion or experimental analysis [3].

This work combines a systematic molecular field analysis of the temperature dependence of the magnetization, and Raman-active spin excitations and phonons coupled to the magnetic structure by the spin-orbit mediated spin-phonon coupling. The use of a comprehensive molecular field model enabled to disclose remarkable magnetic interactions, namely the increase of Fe-sublattice magnetization and its interaction with the R-sublattice [3]. These were seen to be distinctly mirrored by the anomalies in the temperature dependence of Raman-active magnons and the FeO_6 octahedral rotation mode frequency, the later via spin-phonon coupling. This coupling also allows to unravel the distinct magnetic interaction between both Nd^{3+}/Tb^{3+} and the Fe^{3+} spin sublattices through the anomalies observed in the temperature dependence of the corresponding rare-earth oscillations, ascertained to be coupled with the FeO_6 octahedra rotational modes. Contrarily, such anomalous features are not shown in the temperature dependence of both Eu^{3+} and Gd^{3+} oscillation modes, the later due to the lack of spin-orbit coupling. The work here reported provides significant experimental evidence, in a specific set of $RFeO_3$, regarding the Fe^{3+} spins structure below room temperature, its interaction with the rare-earth spins sublattices, and its magnetostructural coupling and gives a renewed overview concerning the mechanisms underlying the complex magnetic properties of $RFeO_3$.

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O24 - HIGH-THROUGHPUT AB-INITIO CALCULATIONS FOR MAGNETO-CALORIC MATERIALS

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The increasing interest in the application of magnetocaloric materials for magnetic cooling devices has led to an intensive search for new materials with a more attractive performance to cost ratio. High-throughput (HT) studies based on first-principles calculations can play a crucial role to detect new magnetocaloric materials and help to estimate trends for material tuning. To identify systems of interest from a large body of data, it is necessary to choose carefully the screening parameters so the accuracy and the cost of the calculations are balanced.

A key quantity to characterize the performance of these systems is the entropy variation between two magnetic phases. In this work, we studied the electronic, structural and magnetic properties of bulk FeRh [1] and Gd from first principles aiming to find a reliable non-tailored approach to determine the entropy variation of the magnetocaloric effect. The calculated entropy values are in good agreement with experimental results for the total entropy [2][3], inspiring the development of a HT workflow.

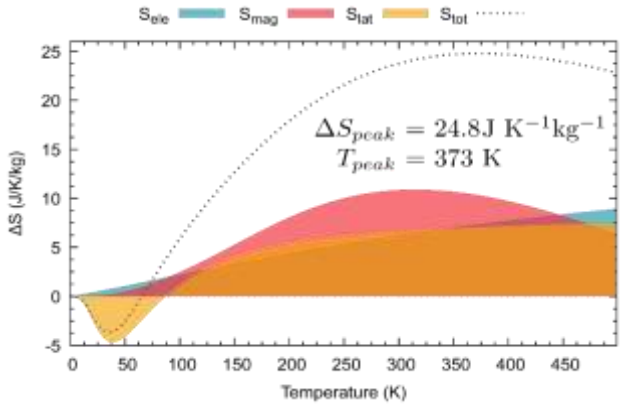

Figure 1. Total entropy variation and respective components estimated for the AFM → FM transition on FeRh [1].

Acknowledgements

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O25 - CONTRACTION AND GIANT NEGATIVE THERMAL EXPANSION AT THE NANOSCALE IN THE $Gd_5(Si,Ge)_4$ MULTIFUNCTIONAL MATERIALS

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The $Gd_5(Si,Ge)_4$ family of compounds is well known for its strong spin-lattice interplay and consequent giant magnetocaloric effect. Recently, micro and nanostructuring $Gd_5(Si,Ge)_4$ studies have been performed with a two-fold motivation: understand size-confinement effects on their properties and broaden their applications towards micro and nano-devices for refrigeration and energy harvesting. In this work, we have investigated the atomic and magnetic structures changes induced by sizeconfinement on $Gd_5(Si,Ge)_4$ nanoparticles produced by pulsed laser ablation. In particular, the atomic structure of 80 nm diameter nanoparticles of $Gd_5Si_{1.3}Ge_{2.7}$ were thoroughly characterized as a function of temperature (synchrotron x-ray diffraction) which unveiled a unique behavior – a negative thermal expansion, in contrast with the positive thermal expansion observed in its bulk counterpart (Figure 1) [1]. This effect emerges because of dimensional confinement and is inherently different from other magnetic nanogranules, suggesting an interplay of different underlying mechanisms, such as the nanoparticle intrinsic surface stress. In addition, three nanoparticles ensembles with different $Gd_5(Si_{1x}Ge_x)_4$ compositions were also studied. For this set of nanoparticles, a unit cell contraction (in comparison bulk) was observed at room-temperature, which imparted a change of their magnetic transition nature from first to second-order [2]. Interestingly, their unit cell contraction was different for different compositions and was shown to correlate with their individual bulk compressibility values. Such correlation suggests that size-confinement, via surface stress, mimics the effects of an external applied pressure.

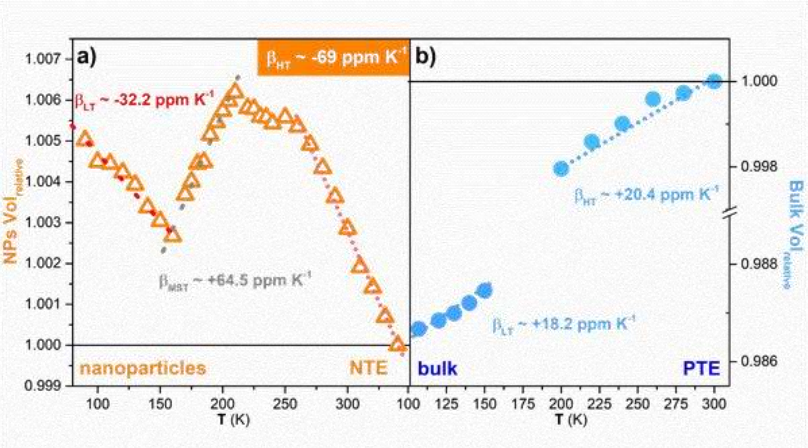

Figure 1. a) Temperature dependence of the unit cell relative volume of $Gd_5Si_{1.3}Ge_{2.7}$ nanoparticles (orange triangles in a), normalized at T = 340K) and of $Gd_5Si_{1.3}Ge_{2.7}$ bulk (blue circles in b)) as a function of temperature.

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O26 - INSIGHTS AND CORRELATIONS BETWEEN EFG AND SPONTANEOUS ELECTRIC POLARIZATION IN HIF MATERIALS

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The relation between electrical polarization and EFG tensors can help in the analysis of experimental results and also provide a better understanding of the phase transitions in ferroelectrics [1,2]. In general, the main EFG component (V_{zz}) is either proportional to squared polarization (P^2) at sites with inversion symmetry in a paraelectric structure, as in $NaNO_2$ [3-5] or proportional to polarization (P) at sites without inversion symmetry [6]. Theoretically, an ab initio study showed a quadratic dependence for proper perovskite ferroelectrics [7]. Recently, perturbed angular correlation (PAC) spectroscopy combined with density functional theory (DFT) calculations were able to investigate how the EFG changes with the ferroelectric phase transitions. However, in hybrid improper ferroelectric (HIF) materials this relation is not clear because the trilinear coupling requires a large set of atomic distortions.

We advance this research by unravelling the relations between V_{zz} and spontaneous polarization in the more complex HIF with the Ruddlesden-Popper (RP) phase and A-site ordered double perovskites (DP) structures. Here, we performed DFT calculations on RP phases $A_3B_2O_7$ and $AA'_2B_2O_7$ and on DP superlattices $AA'B_2O_6$ with A/A' = Ca, Cd and B = Ti, Mn. We showed that for HIFs, quadratic dependency is always found, both for sites with and without inversion symmetry.

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POSTER COMMUNICATIONS SESSION A

A1 - SELECTIVE CONTACTS FOR VERY HIGH EFFICIENCY SOLAR CELLS

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Today, most commercial crystalline silicon with conventional diffused junctions reached upper conversion efficiencies around 22 %, due to recombination losses at the top and bottom contacts. This barrier for conversion efficiency increase is being actively researched and passivation contacts [1] demonstrated the capability to overcome the efficiency bottleneck related to recombination. Although point contacts were also used to try to reduce the recombination, a big advantage of passivating contacts is that they can passivate the entire surface of the wafer instead of localized regions, which has huge advantages regarding manufacturing costs.

The current study shows the progress in the development of SiO2/TiO2 passivating contacts for advanced silicon solar cells to enable very high efficiency conversion. This selective contact requires a tunnel effect layer that reduces recombination at the Si-SO2 interface and at the same time allows electrons to pass across the tunnel layer. So in fact, the TiO2/SiOs stack acts as an electron selective contact.

To obtain a SiO2 layer in the order of 2 nm, we have explored both high and low temperature routes to form this thin SiO2 layer. In the high temperature route, the silicon oxide is obtained by thermal oxidation and in the low temperature route, the silicon oxide is obtained by chemical oxidation or by e-beam evaporation. Several test oxidations were conducted to validate the simulation predictions for equivalent conditions on silicon (100) and compared with elipsometry measurements for experimental validation.

Symmetrical silicon samples with TiO2/SiO2 stacks on each side were prepared and minority carrier lifetimes were measured, to assess the passivation properties of the contacts. It was observed that the high temperature route induces lifetime degradation in the bulk of the wafer and an optimum TiO2 thickness, to minimize contact recombination, was obtained for the chosen SiO2 layer thickness.

Acknowledgements

The authors would like to acknowledge the financial support of FCT through projects: UIDB/50019/2020 – IDL and PTDC/CTM-CTM/28860/2017.

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A2 - IN-SITU CHARACTERIZATION OF PROTON-IRRADIATED CIGS SOLAR CELLS

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CIGS solar cells are a promising power source in harsh radiation environments, due to their ability to recover from radiation-induced damage under certain illumination and temperature conditions and to keep a consistently high output for long periods of time. [1]

At the Laboratory of Accelerators and Radiation Technologies (LATR-CTN), an electro-optical characterization setup has been developed and installed at the 3 MV Tandem ion accelerator, enabling the in-situ measurement of the IV characteristics of CIGS solar cells during irradiation in the dark and under illumination.

Preliminary tests conducted for irradiations with 1 MeV and 2 MeV protons show an overall degradation of the cell performance with increasing fluence, reflected in the reduction of both the open-circuit voltage and fill factor. A significant evolution of the IV curves observed in the minutes following the irradiation evidences a metastable nature of the defects induced in CIGS and suggests that the properties of the pre-irradiated cell can be partially recovered at room temperature.

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A3 - NANOIMPRINT AS A LARGE-AREA NANOFABRICATION TECHNIQUE FOR NANOSTRUCTURED POINT CONTACTS IN ULTRATHIN SOLAR CELLS

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Cu(In, Ga)Se_2 (CIGS) solar cells have the highest efficiency value in thin-film technology (23.35%) [1]. Nevertheless, to reach a bigger expression in the PV market, a reduction in fabrication costs is required, which can be achieved by reducing the CIGS thickness to a sub-micron range. Though ultrathin CIGS presents as an excellent PV candidate, a main limitation is high interface recombination in the rear contact [2]. One strategy to minimize such demise is to implement a nano-patterned dielectric layer between CIGS/rear contact, a solution also called point contacts. So far contacts have been pattern either by high-resolution electron beam lithography (EBL), which is expensive and slow, or by optical lithography- low resolution. Nanoimprint lithography (NIL) presents as a technique that can overcome both techniques.

This work explores the capabilities of NIL and EBL, to pattern rear passivated ultrathin CIGS based devices. NIL was also used to pattern 150x150 mm flexible steel substrates from an industrial scale (Fig. 1). Solar cells patterned with NIL and EBL, both had efficiency values of 12 %. The flexible device was compared to a standard solar cell with a Soda Lime Glass substrate, with a minor loss of 1 % in the efficiency value. The difference between the efficiency values comes from the increased complexity of processing flexible substrates and there is the need for optimization in the CIGS growth parameters for steel-based devices. Given the promising results obtained by NIL, new tests with different rear passivation approaches are under study, to decrease rear interfacial losses.

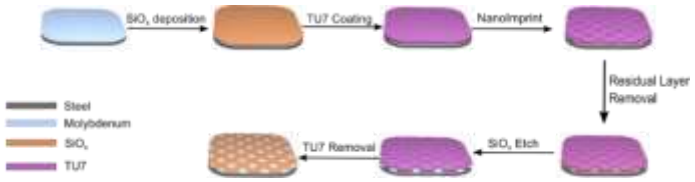

Figure 1 Schematic with the processes step to pattern the large area steel substrates using NIL.

Acknowledgements

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A4 - DEFECT AND STRAIN PROFILES CAUSED BY ION IMPLANTATION IN GaN

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Gallium Nitride (GaN) is a wide bandgap semiconductor, belonging to the III-nitrides family, along with AlN, InN and their ternary and quaternary alloys. It possesses properties, such as high electron mobility, bandgap and electric breakdown field, which allow it to operate under high voltage, high temperature and high frequency regimes without sacrificing its characteristics. This makes GaN an ideal candidate as the next generation replacement of the common Si devices, namely in the field of power electronics. In order to manipulate some of the crystals' properties, ion implantation is often performed. Despite its advantages, this technique creates a lot of defects and strain in the materials, which may hamper proper device operation and reduce its efficiency. In this work, techniques such as Rutherford Backscattering Spectrometry in Channeling mode (RBS/C), and X-Ray Diffraction (XRD) are employed in order to obtain the defect and strain profiles in ion implanted GaN, for several different fluences. The former were extracted from RBS/C using analytical models and MC simulations. These profiles agree well, and are consistent with the strain profiles extracted from XRD in the low fluence range. For high fluences, damage and strain profiles become more inhomogeneous, and results suggest the transformation of defects from point-defects to more complex defects structures. This process leads to stress/strain relaxation, as it was also observed for *in-situ* bending experiments.

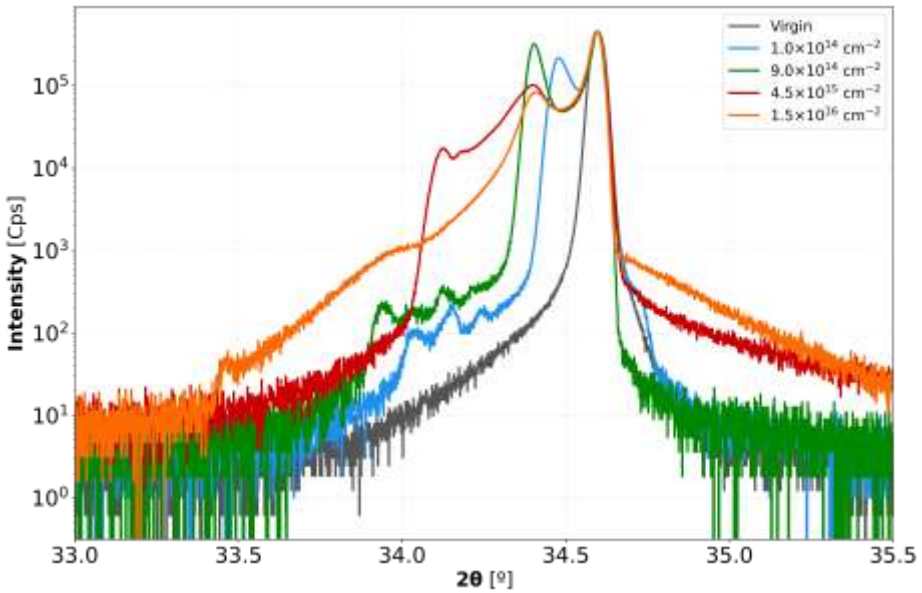

Fig. 1. Experimental XRD pattern for the 002 reflexion of Silicon implanted Gallium Nitride for several different fluences.

A5 - IMPACT OF ANNEALING TEMPERATURE ON STRUCTURAL AND OPTICAL PROPERTIES OF Ga_2O_3 THIN FILMS DEPOSITED USING RADIO FREQUENCY MAGNETRON SPUTTERING

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Gallium oxide (Ga_2O_3) has been a subject of interest as a new semiconductor [1]. The material becomes a very competitive candidate for next-generation electronic devices [2]. Radio Frequency Magnetron Sputtering was employed to deposit Ga_2O_3 on c-plane sapphire (Al_2O_3) substrates at room temperature. The films were annealed at 600, 800, and 1000 °C for 1h in air and post-growth annealing effects of Ga_2O_3 properties were investigated. Optical spectroscopy was performed to evaluate the band gap that varies between 4.44 eV and 4.75 eV for the as-grown and annealed films, depending on the sputtering power and annealing temperature as shown in figure 1. An increase of the optical band gaps has been observed with increasing annealing temperature. In addition, X-Ray Diffraction suggests that the film structure changes from amorphous to crystalline after annealing. The films deposited on Al_2O_3 samples at various sputtering power are pure β-Ga_2O_3 with (100) preferred orientation similar to the sputtering target. Furthermore, Rutherford Backscattering Spectrometry measurements were performed to confirm the stoichiometry of the thin films and to provide the thickness of the Ga_2O_3 thin films. The growth rate for Ga_2O_3 thin films deposited on Al_2O_3 substrates is seen to increase linearly from 0.08 nm/s to 0.16 nm/s as the sputtering power changes from 50 W to 90 W.

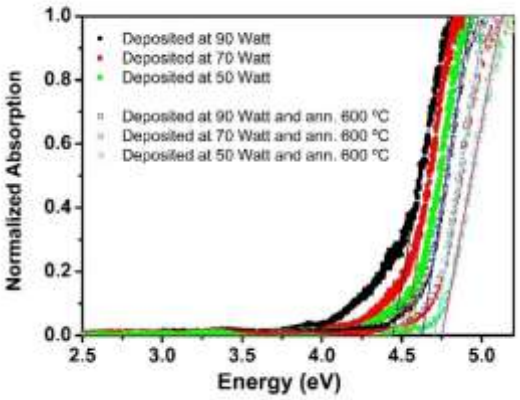

Figure 1. Variation of the normalized optical absorption with photon energy (hν) of as-grown samples and annealed ones at 600 °C. The full line corresponds to the fit of the linear part of the absorption spectra.

Acknowledgements

The authors acknowledge the support from the project funded by FCT. Ref: (CERN/FIS-PAR/0005/2017).

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A6 - OPTICAL BAND GAP OF *h*-$LuFeO_3$ THIN FILMS DEPOSITED BY MOCVD

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The Lu-Fe-O system has several phases with technological interest, such as the $Lu_3Fe_5O_{12}$ garnet, the orthorrombic *o*-$LuFeO_3$ perovskite and the hexagonal *h*-$LuFeO_3$ [1]. The latter is a ferroelectric metastable phase with a theoretical direct bandgap around 1.8 eV which makes it promising for photovoltaic ferroelectric applications. So far only a few reports of band gap measurements in *h*-$LuFeO_3$ thin films are available [2].

In this work, thin films of the Lu-Fe-O system were deposited on silica glass and on (Si(100)/SiO_2/TiO_x/Pt) substrates by Aerosol-assisted Metalorganic Chemical Vapour Deposition (MOCVD). $Lu(tmhd)_3$ and $Fe(tmhd)_3$ were used as metalorganic precursors.

As the *h*-$LuFeO_3$ is a metastable phase, different deposition temperatures (600-800°C) were tested. We concluded that the development of the *h*-$LuFeO_3$ phase is best achieved performing a deposition of an amorphous film at 700°C and latter inducing the crystallization of the *h*-$LuFeO_3$ phase by an *ex-situ* thermal treatment at 850°C. The deposited films were characterized by X-ray diffraction, scanning electron microscopy (SEM) with EDS, atomic force microscopy (AFM), Raman spectroscopy and by optical techniques (UV-Vis). This latter technique allow us to calculate the thickness of the film deposited on silica glass (183 nm) and calculate the direct and indirect optical band gaps, applying Swanepoel and Tauc models respectively to the transmittance spectra. Values of 1.80 eV for direct band gap and of 0.94 and 1.80 eV for indirect band gap were obtained. These values agree with the ones pointed out by Holinsworth [2]. The lowest value (0.94 eV) can be related to the phonon energy.

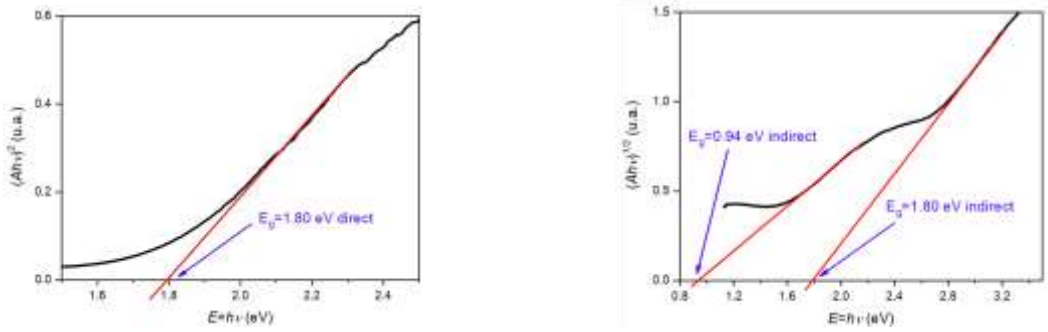

Figure 1. Tauc plots for a) direct bandgap and b) indirect bandgap determination.

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A7 - ACTIVATION OF THE Cr^{3+} LUMINESCENCE IN PROTON-IRRADIATED β-Ga_2O_3

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β-Ga_2O_3 is an emerging wide band gap semiconductor with promising applications. Due to its high transparency (wide band gap of ~ 4.9 eV at room temperature), it is a good host material for optically active centres in the spectral region spanning from the infrared (IR) to the ultraviolet (UV). In particular, besides the intrinsic UV/blue luminescence of undoped β-Ga_2O_3, Cr doping provides efficient red/IR light emission due to Cr^{3+} intraionic transitions. In this work, the dependence of the optical properties of Cr-doped β-Ga_2O_3 single-crystals codoped with Si or Mg with ion irradiation fluence was studied. Iono- and photoluminescence spectra of pristine Si-codoped samples were observed to be dominated by the intrinsic ultraviolet/blue emission; after ion irradiation, this emission is quenched and the Cr^{3+} luminescence is enhanced. On the contrary, for Mg-codoped samples, the Cr^{3+} emission yield is already high in the pristine sample, and no further increase occurs during ion irradiation. Thermoluminescence (TL) measurements, monitored at the Cr^{3+} emission wavelengths, were performed on Si-codoped samples, revealing no signal prior to the ion irradiation. TL was activated after ion irradiation and quenched after annealing at 923 K. X-ray absorption near edge structure measurements show that the Cr ions are mostly in the 3+ charge state before and after irradiation, disproving the hypothesis that the Cr^{3+} emission is enhanced due to a change of the Cr charge state. Alternative mechanisms, including charge/energy transfer paths involving defects, will be discussed. This study thus contributes to a better understanding of the defect levels that can act as sensitisers for Cr^{3+} luminescence in β-Ga_2O_3 and reveals the potential of Cr-doped β-Ga_2O_3 for optical detectors of ionising radiation, both *in*- and *ex-situ*.

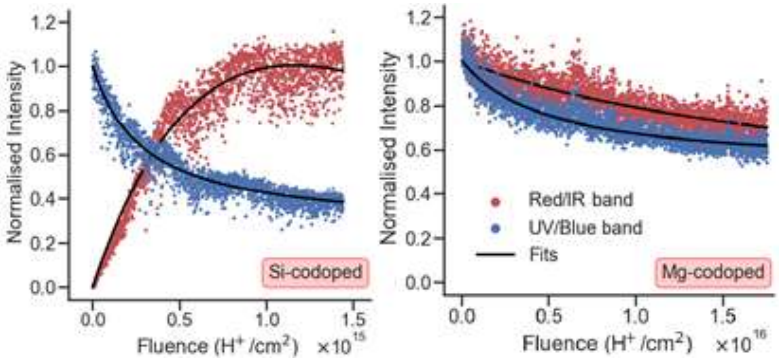

Figure 1. Normalised integrated ionoluminescence intensity of the UV/blue and red/IR bands for Si- (left-hand side) and Mg-codoped (right-hand side) β-Ga_2O_3 irradiated with 600 keV H^+.

Acknowledgements

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A8 - ENHANCED LUMINESCENCE AND OVERCOME OF POLYTYPISM IN Si DOPED GaAs NWs

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The unique properties of semiconductor nanowires (NWs) give these nano-building blocks an outstanding potential for electronic, photonic, mechanical, biological, and energy-conversion applications. It is well-known that GaAs NWs optical and electrical properties are strongly influenced by the simultaneous occurrence of zinc-blende (ZB) and wurtzite (WZ) crystalline structures along the NW's axis. Doping is another crucial issue for NWs applications. In this work, we study the effect of Si doping on the electronic structure of GaAs NWs grown on GaAs (111)B substrates by molecular beam epitaxy, with four nominal Si doping levels (nominal free carrier concentrations of $1x10^{16}$, $8x10^{16}$, $1x10^{18}$ and $5x10^{18}$ cm^{-3}. Using several techniques such as: X-ray diffraction, cathodoluminescence, transmission electron microscopy and photoluminescence, we demonstrate that the presence of fluctuating potentials for the samples with high doping levels, drastically decreases the influence of polytypism on the electronic structure. Such decrease prevents the localization of charge carriers at the WZ/ZB interface. Furthermore, these modifications induced by the increase of the doping level are deeply discussed in the scope of the fluctuating potentials model. The electronic structure of highly Si-doped GaAs NWs as well as the observed increase of the luminescence intensity open up new optoelectronic applications based on III-V NWs.

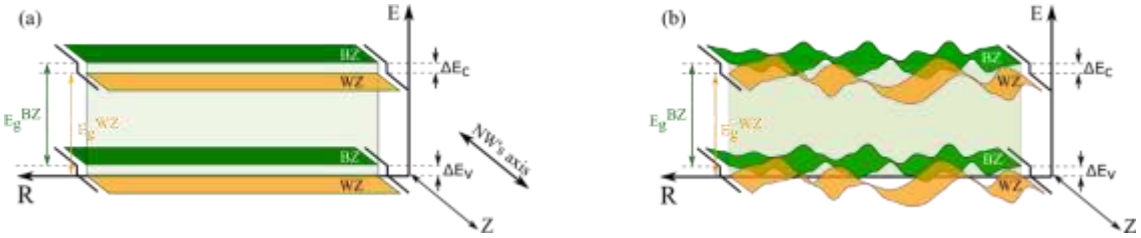

Figure 1. Electronic structure of (a) lightly doped and (b) highly compensated Si-doped GaAs

NWs. Z represents the growth direction of the NW whereas R is an arbitrary radial direction perpendicular to the Z axis. ΔE_c and ΔE_v are the conduction and valence band offsets at the WZ/ZB interface, respectively, in the lightly doped GaAs NW.

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A9 - DISENTANGLING THE PHASE SEQUENCE AND CORRELATED CRITICAL PROPERTIES IN $B_{0.7}La_{0.3}FeO_3$ BY STRUCTURAL STUDIES

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Bismuth ferrite is one of the few room temperature magnetoelectric multiferroics exhibiting simultaneous magnetic and polar ordering at room conditions. But due to its antiferromagnetic character and spiral spin cycloidal structure with an incommensurate modulation wavelength of 62-64 nm, bulk BFO shows very low magnetoelectric coupling. Substitution at the Bi site, especially by La has been reported to show improved magnetic and electric properties due to the effective suppression of the spin cycloid structure and leakage currents. Previous works have shown that $Bi_{0.7}La_{0.3}FeO_3$ is both ferromagnetic and ferroelectric at room temperature [1]. But, there are contradictory reports on the crystal structure [2] and origin of modulation of this composition and further detailed studies were performed to understand the complex physics behind the same.

In this work we have studied the high temperature phase sequence of $Bi_{0.7}La_{0.3}FeO_3$ (BLF30) using high resolution powder neutron diffraction (NPD) and Raman spectroscopy as a function of temperature. Calculation of lattice parameters and modulation wave vector were performed by Pawley refinement of the NPD data. The analysis revealed that BLF30 exhibits an incommensurately modulated orthorhombic P$n2_1a(00\gamma)000$ phase at room temperature. Above T_1 = 543 K, the low temperature modulated P$n2_1a(00\gamma)000$ evolves monotonically into a fractional growing P*nma* structure up to T_N = 663 K. At 663 K, the low temperature canted antiferromagnetic phase is suppressed concurrently with the switching of the former onto a non-modulated P$n2_1a$ structure that continues to coexist with the P*nm*a one, until the latter reaches a 100% fraction of the sample volume at high temperatures above 733 K. Raman mode frequencies also revealed anomaly at these temperatures.

Neutron diffraction and Raman results provide adequate evidence for the existence of a spin-phonon coupling in BLF30. Magnetoelastic coupling is observed below to T_N, involving the canted antiferromagnetic ordering of the spin irons and the symmetric stretching mode of FeO_6 octahedra. The correlation between magnetic data from VSM measurements and the structural results from NPD provides a definite evidence for the magnetic origin of the modulation. The fits to the temperature dependent magnetization from VSM, and the intensity of the magnetic peaks obtained from NPD experiments revealed a critical exponent (β) value of 0.38. The lower limit T_1 = 543 K of the phase coexistence temperature marking the emergence of the P*nma* phase, is also associated with the temperature wherein the modulation magnitude starts to decrease.

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A10 - EFFECTIVE FORCE FIELD CALCULATION FOR THE INTERACTION BETWEEN TWO OPTICALLY HEATED JANUS PARTICLES

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In recent years there has been an increasing research effort, inspired by biological molecular motors, to construct artificial devices which deliver mechanical work or propel themselves in a liquid environment. New strategies showed that a micron-sized Janus particle, half-coated by gold and suspended in a near critical water-2,6 lutidine mixture self-propels after illumination with green light of low intensity [1, 2]. The origin of the active motion relies on the local demixing of the binary solvent observed around the Janus colloid after illumination by light of enough intensity, such that the golden cap is heated above the lower critical temperature of the solvent. Here, we attempt to uncover the basic mechanism for the interaction of light-activated Janus colloids, where the temperature gradient is relevant, through solving, numerically, a purely diffusive and hydrodynamic model [3, 4], and map the effective propulsion force and particle's interaction. We propose a first-generation effective potential that could be used, by the community, for more coarse-grained models (like Langevin Dynamics).

Acknowledgements

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A11 - EXPLORING SOFT MATTER MECHANICS WITH A GENTLE PROBE

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During the last decades, scanning probe microscopies, in particular, atomic force microscopy (AFM) has been playing a major role in exploring the extremely small. In biochemistry and biophysics, its potential was recognized to study interactions between proteins at the single molecule level and to explore the mechanics of living cells. There are, however, several bottlenecks that are particularly unbefitting when measuring a sample's mechanical properties. On the other hand, the effects of mechanical interactions are determinant in a number of cell aspects: mechanotransduction, locomotion, focal adhesion, morphogenesis, apoptosis, disease progression, metastasis, drug cell interactions, etc. From an experimental perspective, there are many techniques focusing on mechanobiology but these often provide contradicting evidence. This work focuses on the implementation of one accurate and reliable method for probing the mechanical response of soft systems. The methodology, nicknamed Gentle Probe (GP) [1], allows to measure the mechanical properties without contact and is consequently insensitive to adhesion forces that mask mechanical properties in conventional AFM experiments. The technique is inherently dynamic, sensitive to the sample's frequency response, robust, and self-calibrating. In GP a spherical probe oscillates in liquid in the vicinity of a deformable object. The pressure modulation of the volume confined between the probe and the object depends on the objects' mechanical response. It turns out that there is a clear critical distance below which the sample response is relevant. This critical distance very sharply depends on the sample's mechanical properties and is readily measurable [1]. If GP is combined with Force Feedback Microscopy [2] then, the method only requires knowledge of the probe size and viscosity of the liquid. Astonishingly it does not require knowledge of the lever transfer function, nor even of the cantilever spring constant.

Acknowledgments

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A12 - SOLUTE TRANSPORT AND DISSOLUTION IN POROUS MEDIA WITH SWELLING

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Transport in porous materials is a problem of relevance for several real-life applications such as disintegration of pharmaceutical tablets, groundwater contamination, and oil extraction. In several cases the fluid modifies the medium, which feedback into the fluid flow. Examples are the erosion and swelling, which greatly impact the fluid dynamics in the porous medium [1]. Here, we study the dissolution and dispersion in a porous medium that swells. We use the Lattice-Boltzmann Method to resolve the fluid flow coupled to an advection-diffusion equation for the solute, to obtain the velocity field and solute concentration. The dissolution causes a solute flux through the surface of the obstacles [2]. The obstacles can either be an infinite or finite source of solute. The implementation of the obstacle swelling is based on the discretization of an empirical law [3] consisting of an exponential increase of the obstacle volume. When the obstacles swell the velocity field decreases for a constant pressure drop and the surface area of the particles increases. We investigate the impact of these factors on the extracted solute over time and determine a macroscopic equation that describes the extracted solute concentration.

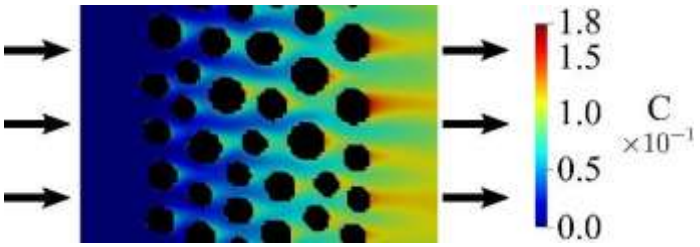

Figure 1. Concentration of solute across the porous medium (colors). The fluid flows from left to right, as shown by the arrows. At the inlet the concentration is fixed at zero and at the outlet we impose an open boundary.

Acknowledgements

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A13 - WOUND OPENING IN A THIN INCOMPRESSIBLE VISCOELASTIC TISSUE

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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 incompressive 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 adimensional parameter, which characterizes the relative importance of viscosity over friction [5].

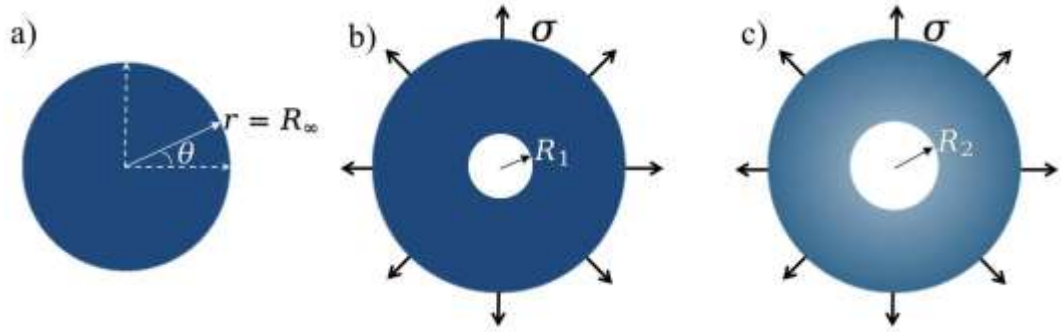

Figure 1. a) A thin circular tissue of radius R_∞ at rest. **b)** The tissue under a uniform radial tension, just immediately after a circular wound of radius R_1. **c)** Final tissue deformation, after relaxation, with a new wound radius, R_2. The colors gradation reflects the intensity of the tissue radial tension.

Acknowledgements

We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under the contracts nº. PTDC/BIA-BID/29709/2017, PTDC/FISMAC/28146/2017, UIDB/00618/2020, and UIDP/00618/2020.

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A14 - MAGNETIC SKYRMIONS IN GaM_4X_8 (M = V, Mo; X = S, Se) LACUNAR SPINELS

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Compounds GaM_4X_8 (M = V, Mo; X = S, Se) belong to the family of lacunar spinels and display many interesting properties correlated with the presence of the Jahn-Teller (JT) effect, a geometric distortion associated with lifting of the degeneracy of the ground-state electron configuration that lowers the energy of the crystal structure when it changes from cubic $F4\#3m$ to rhombohedral $R3m$ space group [1]. These compounds order magnetically at $T_C < T_{JT}$, depicting a ferro/ferrimagnetic behaviour with a saturation magnetic moment at 2 K of ~0.7μ_B/f.u. and ~1μ_B/f.u. for the V and Mo compounds, respectively.
However, the magnetic phase diagram of these compounds is complex, featuring modulated magnetic phases of the cycloidal type and, most remarkably, the presence of magnetic skyrmionic textures has been observed to be stabilised by applying a small magnetic field close to the magnetic ordering temperature [2,3]. Skyrmions are swirling spin structures carrying a topological quantum number and they occur due to the competition between the ferromagnetic exchange and Dzyaloshinskii–Moriya interactions. Their stability, and easy manipulation with small magnetic fields, turn skyrmions into promising candidates for nanotechnological devices, such as data storage systems.
In this work, we will present and discuss the synthesis, structural characterisation, DC/AC magnetic studies and specific heat measurements for the GaM_4X_8 (M = V, Mo; X = S, Se) lacunar spinels. The region of the (H,T) phase diagram where the skyrmionic phases occur can be detected in such compounds by two characteristic anomalies (Fig. 1) observed in dM/dH curves below T_C. For the $GaMo_4S_8$ compound we have also found evidence for spin-glass behaviour in the low-field region of the (H,T) phase diagram close to T_C.

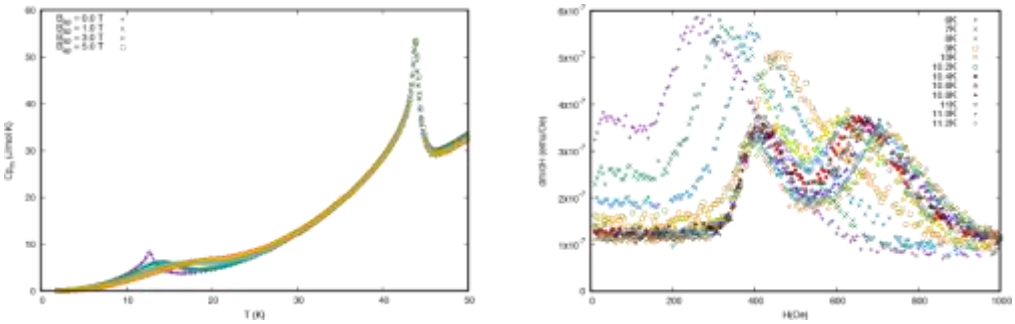

Figure 1 Cp (left) and dM/dH (right) of GaV_4S_8 depicting the JT and magnetic transitions at 43 K and 12.7 K, respectively, and the signature of the skyrmionic phase present close to T_C for fields between 300 and 800 Oe.

Acknowledgments

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 funded under QREN-Mais Centro project 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 and UIDP/FIS/04564/2020.

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A15 - COLLOID-SKYRMION COUPLING – A PATCHY PARTICLES APPROACH

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Recently, a novel class of soft active matter has been realized experimentally [1], topological solitons in confined chiral liquid crystals (LCs), named "skyrmions". Skyrmions are continuous, but topologically protected localized configurations of the LC director field, which exhibit very rich emergent collective dynamics brought by external oscillating electric fields. LC skyrmions can entrap and carry colloidal particles, due to an attractive colloid-skyrmion interaction [2]. In the presence of a static electric field, colloid-skyrmion aggregates interact via equilibrium LC-mediated forces and are also subject to thermal fluctuations. The elastic interaction between skyrmions can be tuned from repulsive to attractive by changing the electric field from 2V to 3V, and for the intermediate voltages the interaction energy is of the order of thermal fluctuations. Coexistence of both colloids and free quasi-particles have been suggested to build composite materials [3], where, if the particle size, surface anchoring, and cholesteric pitch are varied, the properties can be fine-tuned to fit the design in mind.

Here, we study the equilibrium properties of these aggregates using both Monte Carlo simulations and Wertheim perturbation theory [4]. We considered each colloidal particle to be composed of a hard sphere decorated with many attractive sites on their surface and skyrmions as spherical particles with two attractive sites that mimic the dipolar interaction. The relative size of skyrmions can be controlled by the pitch to plate distance ratio [5], and we show the effect of the size ratio of skyrmion to colloid on the formed equilibrium aggregates.

Acknowledgements

We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under Contracts no. PTDC/FIS-MAC/28146/2017 (LISBOA-01-0145-FEDER-028146), PTDC/FIS-MAC/5689/2020, CEECIND/00586/2017, UIDB/00618/2020, and UIDP/00618/2020.

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A16 - THE KINEMATICS OF ACTIVE LIQUID CRYSTAL SKYRMIONS

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Skyrmions are particle-like distortions of a vector field characterized by a topology, which confers them stability. These can be created in liquid crystals (LCs) as well as in ferromagnetic materials. Recently, it has been demonstrated experimentally [1] that skyrmions in confined chiral LCs can exhibit translational motion when subject to oscillating electric fields. Despite the growing number of experimental articles reporting on the collective behaviour of active LC skyrmions, theoretical understanding of the basic physical mechanisms that control skyrmion motion and the effective interactions is rather limited. In this work we study both the kinematics of a single skyrmion in time-varying electric fields, and the effective pairwise interactions, by using two complementary approaches. The first one relies on numerical minimization of the corresponding Frank-Oseen free energy. This computationally expensive method renders the complete information about the timedependence of the LC director profile. The second approach is based on a recent work [2] which introduced a coarse-grained model for motion of skyrmions in LCs, which greatly reduces the computational cost to simulate the motion of a single skyrmion. Here we compare the results of the two approaches. The simplified model revealed that the net displacement of the skyrmion during periodic switching of the electric field is ultimately related to the width of an annulus around the skyrmion center where the director twist is localized. Additionally, the desired control over the skyrmion motion is explored by varying the characteristics of the oscillating field. We also discuss the effective pairwise skyrmion interactions as a function of separation and orientation of the center-to-center vector under different parameters of the electric filed. This work lays the ground to model more complex systems, such as the “flocking” behaviour of a large numbers of skyrmions.

A17 - TINY MAGNETIC FIELDS IN PERIODIC INCOMMENSURATE LATTICES

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The introduction of magnetic fields in lattices with periodic boundary conditions poses a challenge because the allowed magnetic fields are typically very large. Furthermore, the standard Peierls substitution [1] used in periodic tight-binding models is usually incompatible with the geometry of the system when the unit cell has some sort of complexity. Both these issues are merely methodological and hence do not carry any physical consequences, but they do limit the practical usefulness of the methods [2]. In this work, we solve both these issues through a specific gauge choice which allows the magnetic fields to be several orders of magnitude smaller and which also makes the Peierls substitution compatible with any arbitrarily complex unit cell in a periodic lattice. We also find some conditions under which the spectrum of the system is independent of its geometry.

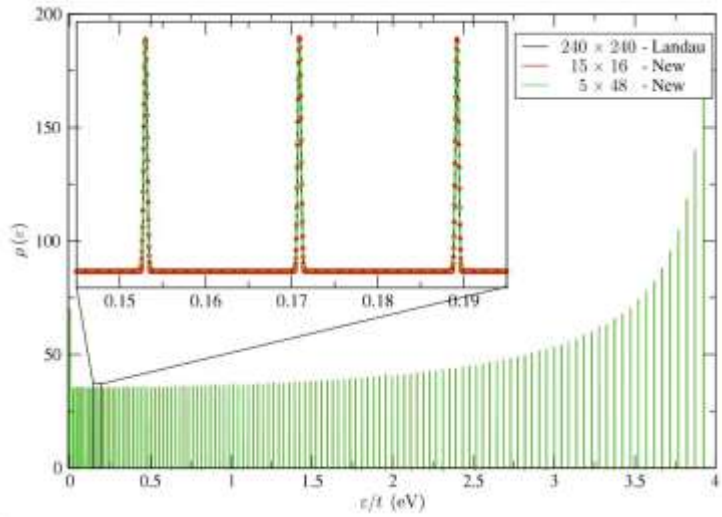

Figure 1: Density of states for the square lattice Hamiltonian for several different geometries. All the curves are identical.

Acknowledgements

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A18 - "FLOCKING" DYNAMICS OF ACTIVE SKYRMIONS

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A novel type of active "particles" realized by topological solitons in confined chiral liquid crystals (LCs) has been recently reported in [1]. These solitons, named "skyrmions" are spatially localized, non-singular configurations of the LC director field that cannot be transformed continuously into a uniform state. The LC skyrmions acquire motion powered by a time-dependent electric field applied to the LC in a direction normal to the confining [1]. The basic physical mechanism of the skyrmion motion is related to the "non-reciprocal" rotational dynamics of the LC director field when the electric field is turned on and off. Recent experimental results [2] reveal rich collective dynamics of thousands-to-millions of active LC skyrmions. Initially, each skyrmion moves in a random in-plane direction, but after a short period of time, of the order of a second, schools of skyrmions moving in the same direction are formed. Experiments emphasise the role of immobile obstacles, such as other skyrmions pinned to substrates using laser tweezers, in the control of the collective dynamics of skyrmion clusters which exchange and rearrange individual skyrmions through the interactions with the obstacles. Here, we develop a particle-based stochastic model, where each skyrmion is represented by a self-propelled particle that moves at a constant velocity, with a coupling between the rotational degrees of freedom, such that each particle tends to align its velocity with the average of their neighbours (Vicsek-like coupling). We introduced a timescale of alignment that can be related with the response of the liquid crystal. We studied how the timescale of alignment and the density of pinned skyrmions affects the asymptotic steady state regime. Furthermore, systems with pinned skyrmions reach the steady state with a partial alignment, which depends both on the density of pinned skyrmions and the timescale of alignment.

Acknowledgements

We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under Contracts no. PTDC/FIS-MAC/28146/2017 (LISBOA-01-0145-FEDER-028146), PTDC/FIS-MAC/5689/2020, CEECIND/00586/2017, UIDB/00618/2020, and UIDP/00618/2020.

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A19 - SHAPE TRANSITION OF FLOWING SKYRMIONS IN 2D

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We investigate, numerically, the effects of externally imposed material flows on the structure and temporal evolution of liquid crystal skyrmions. The dynamics of a 2D system of skyrmions is modeled using the Ericksen–Leslie theory, which is based on two coupled equations, one for material flow and the other for the director field. As the time scales of the velocity and director fields differ by several orders of magnitude for realistic values of the system parameters, we have simplified the calculations by assuming that the velocity relaxes instantaneously when compared to the relaxation of the director field. Thus, we have used a finite-differences method known as artificial compressibility with adaptive time step to solve the velocity field and a fourth-order Runge-Kutta method for the director field. We characterized the skyrmion shape or configuration as a function of the time and the average velocity of the flow field. We found that for velocities above a certain threshold, the skyrmions stretch in the direction perpendicular to the flow, by contrast to the regime of weak flows where the skyrmions stretch along the streamlines of the flow field. These two regimes are separated by an abrupt (first-order) dynamical transition, which is robust with respect to e.g., the LC elastic anisotropy. Additionally, we have found how the presence of a second skyrmion affects the evolution of the shape of the skyrmions, by comparing the evolution of pairs of skyrmions to the evolution of a single-skyrmion. The prediction of the skyrmion shape transition was confirmed experimentally [2].

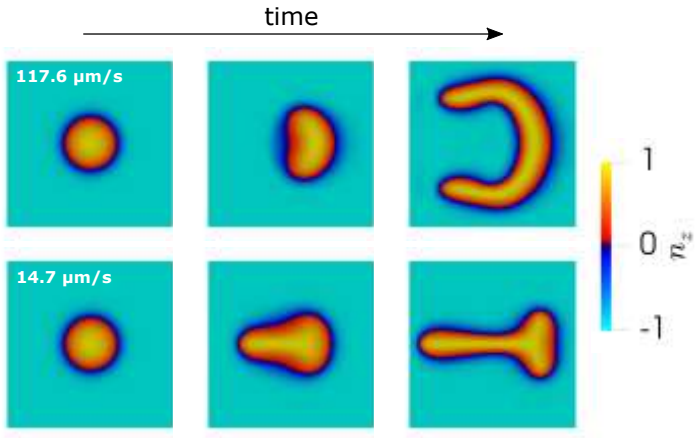

Figure 1. Time evolution of the skyrmion shape for two different velocities.

Acknowledgements

This work was funded by the Portuguese Foundation for Science and Technology (FCT) under the contracts: PTDC/FIS-MAC/5689/2020, EXPL/FIS-MAC/0406/2021, UIDB/00618/2020 and UIDP/00618/2020.

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A20 - MACHINE LEARNING APPROACH FOR COARSE-GRAINED ACTIVE LIQUID-CRYSTAL SKYRMIONS

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Recently, a novel class of soft active matter has been realized experimentally, where topological solitons in confined chiral liquid crystals (LCs), named "skyrmions", are the elementary building blocks of the active matter system [1]. The skyrmions are continuous, but topologically protected localized configurations of the LC director field and are analogs of the Skyrme solitons in nuclear physics. The skyrmions are brought into directed motion by oscillating external electric fields, and exhibit very rich emergent collective dynamics, with no analogs in more traditional passive or active colloids. When the voltage modulation period is shorter than the LC response time, the skyrmion interactions are intrinsically nonequilibrium, resulting in remarkably rich emergent collective dynamics with reconfigurable out-of-equilibrium assemblies of skyrmions.

In this works, we combine Finite Elements Method (FEM) with a machine learning approach. Since FEM results are very sensitive to the spatial arrangement of the skyrmions, we implemented a convolutional neural network (CNN) approach, where a discretized order parameter profile will be passed through convolutional and pooling layers of the CNN whose output will then be fed into the final fully connected layers for final classification purposes.

Figure 1. Example of a polarizing optical microscopy image obtained from finite elements calculations with a corresponding free energy of -0.20402029.

Acknowledgements

We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under Contracts no. PTDC/FIS-MAC/5689/2020, CEECIND/00586/2017.

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A21 - MODELING THE MECHANICAL PROPERTIES OF COLLOIDAL GELS

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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 the rotational degrees of freedom affect 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 were also able to provide us with valuable information on the physical properties of the gel such as the variation of bonds when a shear stress is applied and its viscoelasticity. The latter was computed through passive microrheology using conventional mean squared displacement. Another technique, the two-point microrheology, previously used on image-based particle tracking systems [2] is applied to numerical simulations again to provide insight on the variation of viscoelasticity.

Acknowledgements

We acknowledge financial support 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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A22 - DYNAMICS OF IMMISCIBLE DROPLETS IN A POROUS MEDIA

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The flow of droplets transported by a fluid occurs in different situations, such as in enhanced oil extraction, water filtration and in clinical analyses. Recent microfluidic experiments suggest that deformable particles cooperate with each other through hydrodynamic interactions to pass through a porous medium, for which, under the same conditions, a single particle gets trapped [1]. For a mixture with particles of different flexibilities, we observe that more flexible particles move faster than the less flexible ones. We simulated immiscible droplets passing through obstacles using the lattice-Boltzmann method and studied the interaction between them [2,3]. We describe how the droplets cooperate to pass through the porous medium under conditions when one single droplet would get trapped. We find that the average velocity of the droplets increases with the number of droplets in the medium and they accumulate forming horizontal lines for small inlet velocities.

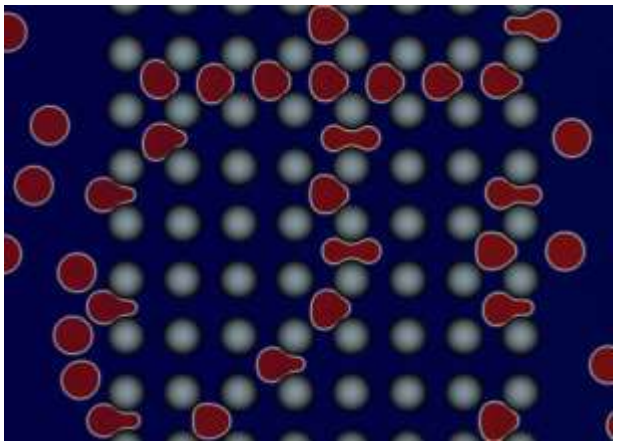

Figure 1. Immiscible droplets (in red) passing through obstacles for a certain time.

Acknowledgements

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A23 - CELLULOSE-BASED LIQUID CRYSTALS FOR 3D STRUCTURAL COLOURED OBJECTS

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Reaction/diffusion mechanisms have been referred in literature to describe the appearance of spots, stripes and other existing patterns in insects, birds and mammals, such as in the cuticle of beetles, in the wings of butterflies and peacock feathers [1]. Some of these patterns exhibit structural colours that give rise to golden and silver reflections. In this work reaction-diffusion mechanisms are used to explain the formation of unusual structural patterns in liquid crystalline cellulose-based structures [2]. 3D printing is used to shape the colored structures into objects that are sensitive to humidity and temperature. The obtained materials colour depends on a helical periodic structure that allows selective reflection of the light. The characterization of the materials involves optical characterization, scanning electron microscopy (SEM), atomic force microscopy (AFM), nuclear magnetic resonance (NMR) and infrared (IR) spectroscopy.

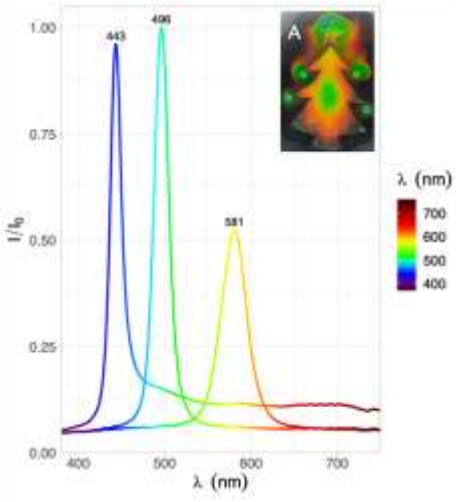

Figure 1. Reflectance spectra recorded at different regions of sample *A* (*A* is a photo of a sample prepared from a lyotropic cellulose liquid crystal, showing a gradient of colours, which arises from variations of the helical pitch of the cholesteric structure).

Acknowledgements

A.A. acknowledges the Minister of Science, Technology, and Higher Education for National Funds, European Social Funds, and FCT for fellowships with reference SFRH/BD/115567/2016. This work is co-financed by FEDER, European funds, through the COMPETE 2020 POCI and PORL, National Funds through FCT – Portuguese Foundation for Science and Technology and POR Lisboa2020, under the projects PIDDAC (POCI-01-0145FEDER-007688, Reference UIDB/50025/2020-2023), PTDC/CTM-REF/30529/2017 (NanoCell2SEC) and Action European Topology Interdisciplinary Action (EUTOPIA CA17139).

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A24 - ANISOTROPIC CELLULOSE-BASED FILMS FOR TIME-TEMPERATURE SENSORS

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Shear-casting techniques are used to produce anisotropic films from cellulose-based liquid crystalline thermotropic and lyotropic systems. The films produced exhibit anisotropic mechanical properties, are ductile when stretched perpendicular to the shear direction and brittle when stretched parallel to it [1]. The anisotropy of the films results from the alignment of the polymeric chains after shear cessation due to the evaporation of the solvent and to the high viscosity of the chains of cellulose. During shear elastic energy is stored in the system leading, after shear cessation, the oriented cellulosic chains to partially relax. The relaxation of the shear- aligned chains is a collective effect due to the fact that the highly concentrated and aligned polymers with sufficiently rigid chains cannot relax individually [2]. The resulting internal stress induces a periodical contraction (bands), often observed after shear (Figure 1). The shear-band texture is ruled by any factors that include the precursor solution composition, solvent evaporation rate, film thickness, rate and duration of shear. In this work we prepared, by shear-casting, films of acetoxy propyl cellulose (APC), the mechanical properties of the films were measured and for a certain constant value of the stress, the lateral dimensions of the sample were recorded in time (Figure 1). The contraction of the sample depends on the value and direction of the applied strain (parallel or perpendicular to the shear-casting) and temperature. The lateral contraction of the sample was attributed to the relaxation of the material that shows a tendency to reform the sinusoidal band morphology.

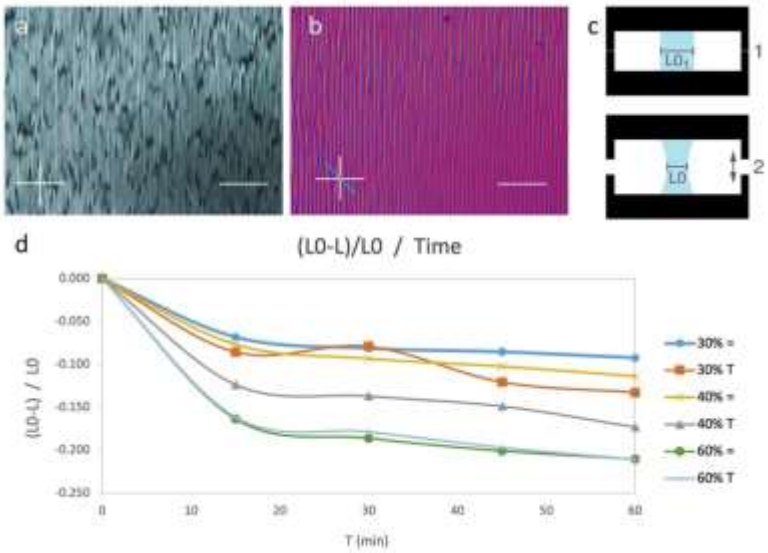

Figure 1: Optical and mechanical properties of a film of APC prepared by shear casting. a. and b. texture of the film after relaxation, between cross polarizers and between cross polarizers and a lambda plate, respectively. c. lateral dimension measurement scheme with initial position (1) and final position (2). d. evolution of the lateral dimensions of the film for 30%, 40% and 60% of stretching.

Acknowledgements

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A25 - BACTERIAL CELLULOSE BASED HYDROGELS FOR WOUND DRESSING APPLICATION

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In the past few decades several approaches were made to provide a better wound healing treatment as new strategies emerge to produce novel types of dressings. It comes as a demand that materials for novel wound dressings not only take an active part in wound protection but also present a set of features that allow and contribute to efficient skin recovery. Therefore, bacterial cellulose (BC), an extremely pure form of cellulose, appears as an attractive biomaterial for advanced wound management due to its unique intrinsic properties such as biocompatibility, non-toxicity, mechanical stability, transparency and high moisture content [1]. To compete with the already existing commercially available products, many approaches can be taken in order to modify BC to address specific applications – individually or in the combination with different components. In burn wound care, the maintenance of an hydrated bed wound and the prevention of infections are key features to reduce treatment length and health related costs. Therefore, *in situ* and *ex situ* modifications have been especially focused in conferring and enhancing BC's antimicrobial activity and water uptake content features. The adaptation of the production conditions and the *ex situ* incorporation of compounds such as metallic nanoparticles, have been linked to a faster tissue regrowth, while being easily accessible and inexpensive, thus providing a better cost/benefit ratio of the dressings and being an environmental friendly alternative to the existing market. The BC membranes were physically characterized in order to infer the influence that each modified parameter has on the BC hydrogel's properties. The membranes were also microbiologically tested to quantify their antimicrobial efficiency.

Figure 1. Hydrated BC membrane collected immediately after production by *K. Rhaeticus*, a non-pathogenic Gram-negative bacteria of the genus *Komagateibacter*.

Acknowledgements

A.A. acknowledges the Minister of Science, Technology, and Higher Education for National Funds, European Social Funds, and FCT for fellowships with reference SFRH/BD/115567/2016. This work is co-financed by National Funds through FCT – Portuguese Foundation for Science and Technology under the projects Reference UIDB/50025/2020-2023 (CENIMAT); PTDC/BIA-MIC/31645/2017 (R.G.S.); and the Applied Molecular Biosciences Unit, UCIBIO, which is financed by national funds from FCT (UIDB/ 04378/2020) and co-financed by the ERDF under the PT2020 Partnership Agreement No. POCI-01-0145-FEDER-007728.

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A26 - DEVELOPMENT OF A MICROFABRICATION PROCESS FOR 3D STAIRCASE STRUCTURES WITH THROUGH-LEVEL ELECTRICAL CONNECTIONS

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3-Dimensional structures for electrodes and other microstructures are of interest for biosensing applications [1], optics [2] and micro-electromechanical systems (MEMS) [3], offering the ability to measure electrical signals at distant heights with precise positioning. In this work, we used direct laser writing lithography to define patterns with different heights by varying the exposure dose. The ma-P 1275 G photoresist, designed for grayscale lithography [2], was chosen due to its low contrast and high viscosity, allowing coating of thick layers. A 10 μm layer was obtained by spin-coating at 3000 rpm for 30 seconds and soft baking at 85 °C for 60 seconds. A Heidelberg DWL 2.0 system with a 90 mW, 405 nm laser was used for exposure. After development, a pattern with 3 steps at distinct heights was obtained. Reactive Ion Etching in an SPTS Omega ICP system was then used to transfer the pattern onto an SiO_2 layer, at 70 mTorr and using 1000 W of source RF power, 200 W of platen RF power, 18.0 sccm of SF_6 and 9.0 sccm of H_2. Figure 1a shows an example of the final structure, with 3 levels at different heights: the first level at substrate surface (0 μm), the second at 1.7 μm and the third at 2.6 μm. The sidewall angles were of 64.0° ± 4.7° between levels 1 and 2, 76.4° ± 1.9° between levels 2 and 3 and 34.6° ± 4.7° between levels 3 and 1. Gold leads were deposited crossing all steps for demonstration of the viability of the process (Fig. 1b), using magnetron sputtering (10 nm Cr adhesion layer, obtained with 20 sccm Ar flow, 20 W of DC power, and 100 nm Au, obtained with 20 sccm Ar flow, 20 W of RF power) and using lift-off to transfer the pattern. Electrical contact between successive levels was achieved, demonstrating the feasibility of the method.

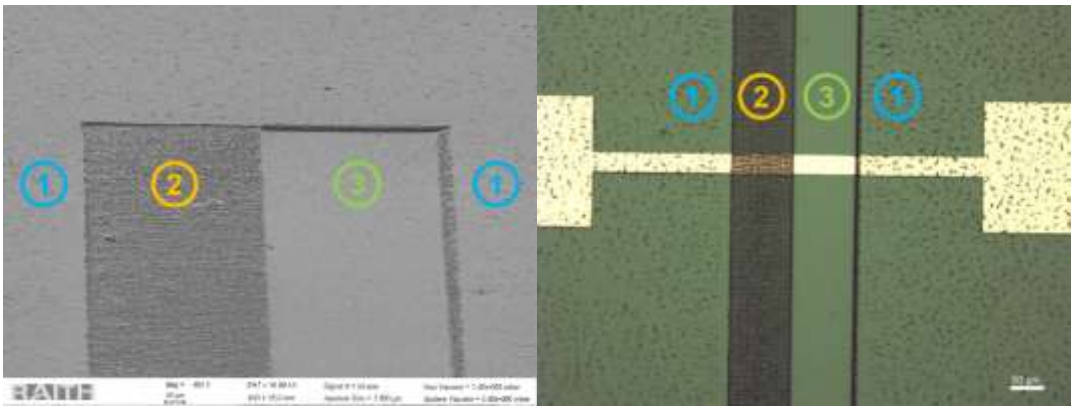

Figure 1. (a) SEM imaging of the multiple levels on SiO_2. **(b)** Au leads crossing several layers. Regions: (1) – SiO_2 height = 2.6 μm; (2) – SiO_2 height = 1.7 μm; (3) – SiO_2 height = 0 μm.

Acknowledgements

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A27 - TWIST AND CURVATURE IN CELLULOSE BASED RIBBONS FROM *ERODIUM* AWNS FOR REMOVAL OF DIES FROM WATER

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A wide diversity of intricate movements, triggered by the variation of humidity, is observed in dead tissues of plants. This is the case of the awns to which the seeds of the *Erodium* plant are attached. The hygroscopic movements of the awns allow the dispersal and the digging of the seeds. The geometrical arrangement of cellulose fibrils on the cell walls of the awns keeps them responsive to humidity even after leaving the plant and the seeds. Dry awns exhibit a right-handed coil, while in the wet state a taut conformation is observed[1]. Lefthanded coils were observed in chemically modified wet awns. In this work chemically modified awns are used as adsorbents for the removal of crystal violet dye from an aqueous solution. The modification based on NaOH and Na_2SO_3 treatment of the awn dead fibers[2] was confirmed by scanning electron microscopy, X-ray diffractometry, Fourier transform infrared spectroscopy and scanning electron microscopy. The dye removal efficiency was evaluated by determining the variation in dye concentration, pH and adsorbent mass. The chirality of the awns allows their cleaning, after adsorption of the dye, in specific solvents.

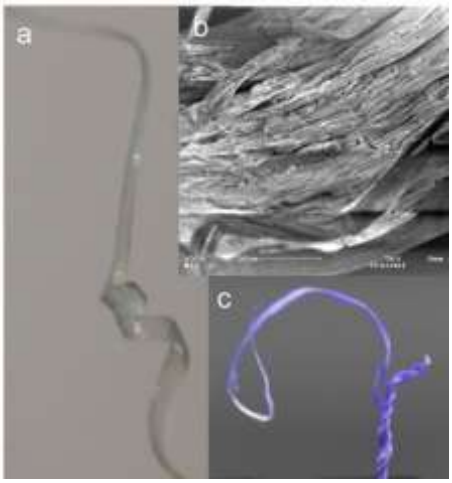

Figure 1. Soft right-handed dry ribbons from the awns of *Erodium*, after chemical treatment. a) Transparent birefringent ribbon. b) Scanning electron photo showing that micro pits existing along the tubular structures of the ribbon in a), were not affected by the chemical treatment. c) Ribbon after being immersed in a crystal violet dye aqueous solution.

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A.A. acknowledges the Minister of Science, Technology, and Higher Education for National Funds, European Social Funds, and FCT for fellowships with reference SFRH/BD/115567/2016. This work is co-financed by FEDER, European funds, through the COMPETE 2020 POCI and PORL, National Funds through FCT – Portuguese Foundation for Science and Technology and POR Lisboa2020, under the projects PIDDAC (POCI01-0145-FEDER-007688, Reference UIDB/50025/2020-2023) and Action European Topology Interdisciplinary Action (EUTOPIA CA17139).

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A28 - OPTIMIZATION OF OUT-OF-PLANE SYNTHETIC ANTIFERROMAGNETIC STRUCTURES WITH IRIDIUM SPACER

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Reference systems in magnetic tunnel junctions with extremely high thermal stability are critical for spin electronic applications - memories [1] and sensing devices [2]. Typically, synthetic antiferromagnetic (SAF) structures based on Ruthenium spacers are used to increase the pinning fields up to a few kOe enhancing the reference stability and reducing errors in the device operation. In these structures, the interfacial physical interactions play a major role reaching the required pinning fields. This work presents the optimization of SAF structures with Iridium spacer recently known to induce a strong antiferromagnetic interlayer coupling [3]. The prepared structures are based in [Co/Pt]/(IrRu)/[Co/Pt] multilayers for achieving out of plane magnetic anisotropy deposited by magnetron sputtering with base pressure of $2x10^{-7}$ Torr. The used spacer is an Iridium rich alloy with following composition: $Ir_{98.7}Ru_{1.3}$. Different spacer thicknesses, buffer layers and SAF multilayer numbers were fabricated to obtain the maximum interlayer exchange coupling. M(H) characterization was done by vibrating sample magnetometry. Typical results are shown in figure 1 where a clear out-of-plane SAF behavior is observed for the magnetic perpendicular anisotropy multilayers coupled via iridium spacer arising coupling fields up to ~5500 Oe. The coupling fields obtained are well suited for out-of-plane sensor applications.

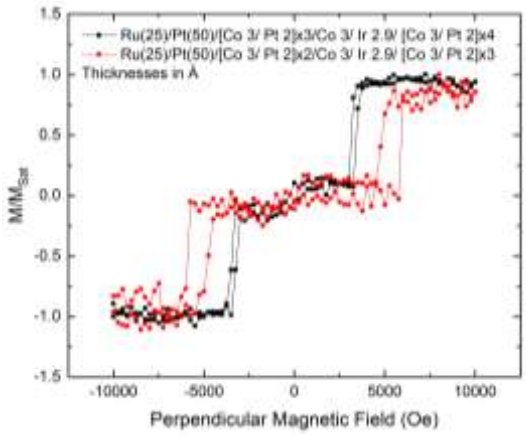

Figure 1. Representative M(H) loops for two SAF structures obtained with Iridium spacer.

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A29 - MECHANICAL PROPERTIES OF HUMAN BRONCHIAL EPITHELIAL CELLS EXPRESSING Wt- AND MUTANT CFTR

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Cystic fibrosis (CF) is caused by mutations in the gene encoding the cystic fibrosis transmembrane conductance regulator (CFTR). A single recessive mutation, the deletion of phenylalanine 508 (F508del), causes severe CF and resides on 70% of mutant chromosomes [1]. Disorganization of the actin cytoskeleton has been previously reported in relation to the CF phenotype. In this work, we aimed to understand this alteration by means of Atomic Force Microscopy and Force Feedback Microscopy [2] investigation of mechanical properties of cystic fibrosis bronchial epithelial (CFBE) cells stably transduced with either wild type (wt-) or F508del-CFTR. We show here that the expression of mutant CFTR causes a decrease in the cell's apparent Young modulus as compared to the expression of the wt protein.

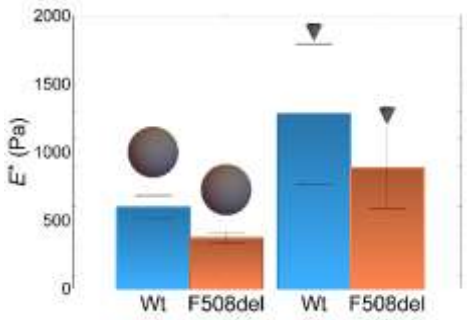

Figure 1. Atomic force microscopy analysis of wt-CFTR and F508del-CFTR cells obtained with Force Feedback Microscopy (FFM) using a spherical 1 μm radius bead and with an Atomic Force Microscopy (AFM) and a pyramidal tip.

Acknowledgements

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A30 - MAGNETITE NANOPARTICLES FOR MAGNETIC HYPERTHERMIA

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Magnetic nanoparticles (MNP) have been investigated for their use in magnetic hyperthermia, a promising technique for cancer treatment, that relies on the optimization of the heating ability of the MNP when exposed to an alternate magnetic field. The specific loss power (SLP), defined as the power dissipated per unit mass of the MNP is the parameter to be optimized.

Although several materials and material combination have been explored for MH, magnetite is still considered the best candidate for the nanoparticle composition due to its biocompatibility and high saturation magnetization. In this work, we explore magnetite nanoparticles synthesized by co-precipitation under an applied dc magnetic field, using a green synthesis method, to produce organized MNPs. The organization was fixed using pectin, later polymerized, allowing for the preparation of water-based suspensions of these nanoparticles.

The particles morphological, structural, and magnetic properties were evaluated and correlated with the SLP values obtained for the water-based suspensions under alternate magnetic fields with 275 kHz frequency and 14 kA/m amplitude.

Acknowledgements

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A31 - EFFECT OF Mn SUBSTITUTION ON THE STRUCTURAL AND MAGNETIC PROPERTIES OF Ca DOPED BISMUTH FERRITE

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Chemical substitution-related strategies to achieve spontaneous magnetization in the multiferroic $BiFeO_3$ exploit the possibility to suppress its cycloidal antiferromagnetic structure in favor of a canted antiferromagnetic one. Herein we explore an alternative approach towards attaining a large switchable magnetization in the ferroelectric compound [1, 2]. We use a doping scheme in which Fe^{3+} ions are partially replaced by manganese in the mixed (Mn^{3+}/Mn^{4+}) oxidation state providing the ferromagnetic exchange coupling. The Ca-doped bismuth ferromanganites

$Bi_{0.85}Ca_{0.15}Fe_{1-x}Mn_xO_3$ ($0.1 \leq x \leq 0.5$) have been synthesized by a solid-state reaction method. It has been found that the increase in Mn concentration induces a modification of crystal and magnetic structures giving rise to the canted antiferromagnetic polar phase → collinear antiferromagnetic polar phase → paramagnetic nonpolar phase transitions at room temperature. The appearance of spontaneous magnetization suggesting a transformation of the collinear antiferromagnetic structure is observed with decreasing temperature. The transformation of the magnetic arrangement can also be driven by a magnetic field application. Such metamagnetic transition can be accompanied by a large (up to ~4 emu/g for the sample with x= 0.4, when measured at T= 2 K) magnetization jump (Fig. 1) far exceeding that specific to a field-driven cycloidal order → canted order transformation in the pure BiFeO3.

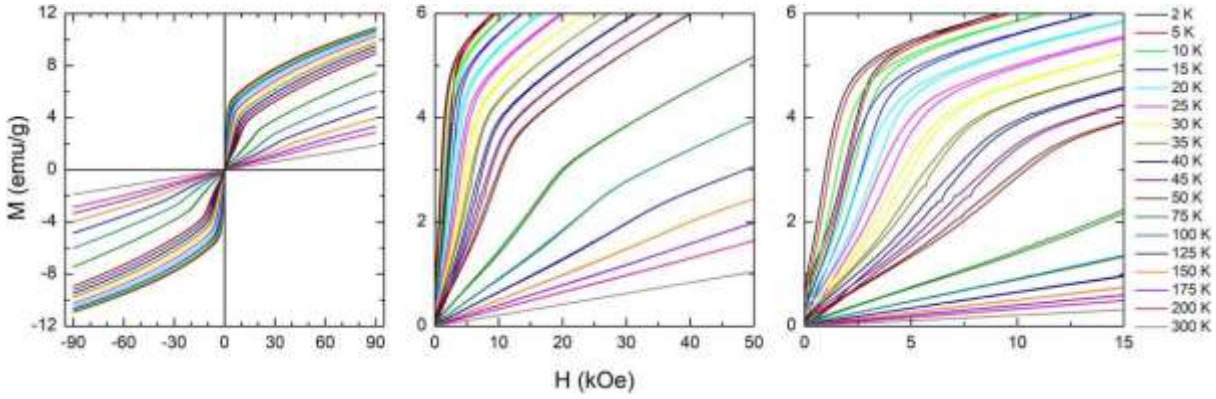

Fig. 1. Field dependencies of magnetization obtained from the sample with x= 0.4 at different temperatures [2].

Acknowledgements

This work was supported by the RSF (project 21-19-00386). Investigations done at the CFisUC were supported by the FCT (projects UIDB/04564/2020 and UIDP/04564/2020). Access to TAIL-UC facility is gratefully acknowledged.

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A32 - CONTROL OF STRUCTUAL AND MAGNETIC PROPERTIES OF POLYCRYSTALLINE Co_2FeGe FILMS VIA DEPOSITON AND ANNEALING TEMPERATURES

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Stoichiometric Heusler alloy (HA) Co_2FeGe (CFG) is half-metallic ferromagnet with high magnetization and Curie temperature which makes it very attractive for spintronics applications. Here we report effects of the deposition (T_S) and annealing (T_a) temperatures on structural and magnetic characterization of CFG films. Films were deposited on Corning Glass substrates using magnetron co – sputtering technique. Films were found to be polycrystalline. Ordered $L2_1$ phase was observed for elevated T_S. Magnetic properties are listed in Table 1. Damping parameter α as low as 0.004 was achieved. Properties of the films could be effectively tuned in a wide range. This paves the way for technological applications.

T_S, K	T_a, K	From SQUID		From FMR		
		M_S, emu/cm^3	H_C, Oe	M_{eff}, emu/cm^3	A, pJ/m	α
RT	---	710	6	738	6.8	0.007
573	---	920	2	895	9.2	0.004
773	---	880	65	930	9.3	0.06
RT	573	870	3	906	9.8	0.005
RT	773	840	6	882	9.4	0.009

Figure 1/Table 1 Deposition temperature (T_S), temperature of annealing (T_a), saturation magnetization (M_S) and coercive field (H_C) determined from SQUID measurements, effective magnetization (M_{eff}), exchange stiffness (A) and damping parameter (α) determined from FMR measurements.

Acknowledgements

Work with support from Network of Extreme Conditions Laboratories-NECL and Portuguese Foundation of Science and Technology (FCT) support through the projects PTDC/FIS-MAC/31302/2017, NORTE-01-0145-FEDER-022096, EXPL/IF/00541/2015 (S.A.B.), SFRH/BPD/84948/2012 (A.V.), and SFRH/BPD/87430/2012 (A.A.).

A33 - NUMERICAL SIMULATON OF A PASSIVE THERMAL SWITCH

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Keeping devices operating at adequate temperatures is necessary for numerous technological areas. One innovative component that can contribute to this control is the thermal switch (TS). TSs rely on the switching of thermal resistance between two states: during the “on” (“off”) state, the thermal resistance is minimized (maximized), thus maximizing (minimizing) heat transfer1. The operation can depend on an external activation source - active TS [1,2] - or only on the atomic structure and thermal properties of the material used as the heat transfer medium - passive TS [3,4]. In this work, we propose a novel passive TS based on shape-memory alloys (SMAs), that does not require energy consumption. With the python-based framework heatrapy [5], we simulated its applicability by mimicking the cooling of an electrical component (*C*). Figure 1 (a) shows the thermal switch in the “on” (martensite) and “off” (austenite) state. It consists of three blocks: the base, the moving part (ts) and an intermediate block (*m*). Due to the existence of four thermal insulators, the temperature of each of the four springs varies only with *ts* and *C* temperatures. We performed simulations for different *base*/*m*/*ts* stacks, starting with *Cu*/*Cu*/*Cu* (Figure. 1 (b)). A period of 0.909 s was obtained. Other stacks were evaluated (Figure 1 (c)), noticing that the period decreases with the increase of the thermal diffusivity.

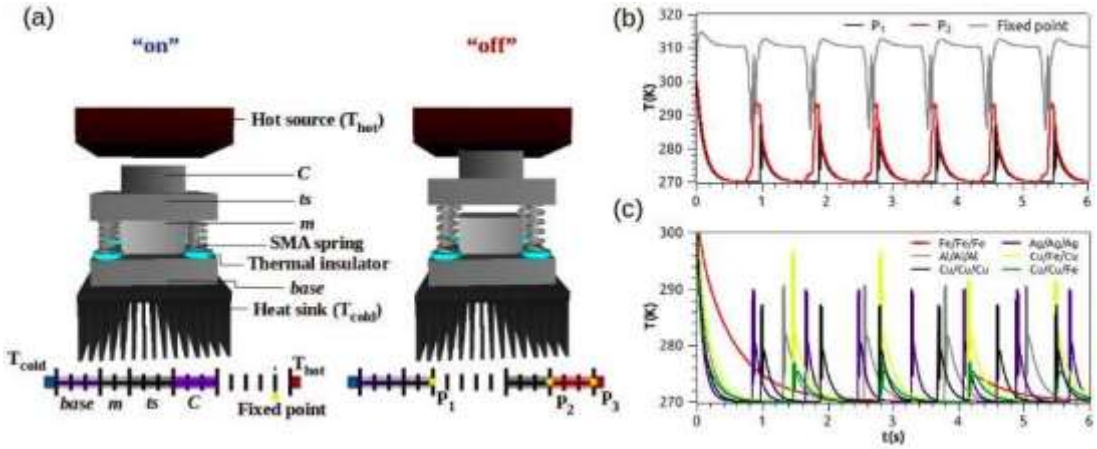

Figure 1. (a) Proposed thermal switch. Periodic behavior of (b) stack *Cu/Cu/Cu* and (c) stacks with different materials.

Acknowledgements

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A34 - PROPERTIES OF Cu-Y_2O_3 AND CuCrZr-Y_2O_3 COMPOSITES AS THERMAL BARRIERS

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The Cu-Y_2O_3 and CuCrZr-Y_2O_3 materials have been devised as thermal barriers. The composites were prepared in a glove box and consolidated with spark plasma sintering between 775-800ºC with pressures of 57 MPa with a holding time of 5-8 min. Moreover, samples were produced by changing the volume fraction of Y_2O_3 (1, 5, 10, and 15 % with Cu and 1, 5, 10, and 15 % with CuCrZr). The microstructure of the consolidated samples revealed dispersions of Y_2O_3 regions in the Cu matrix or in the CuCrZr and Y_2O_3 agglomerates. All the consolidated materials with Cu evidence an oxide formation and the densifications are between 90 to 99% with the decreasing of densification with the increasing of the Y_2O_3 %. Thermal diffusivity of the samples Cu- 5%Y_2O_3 and CuCrZr- 5% Y_2O_3 (with higher densification) are similar, and the values are lower than pure CuCrZr and Cu but higher than W. A ductile behavior was observed in all the temperature ranges, and the samples CuCrZr-based exhibited 6x higher smax than Cu-based material, although this difference was lower as temperature increased.

POSTER COMMUNICATIONS SESSION B

B1 - EXPLORING NEW ELECTRONIC PHASES IN THE HONEYCOMB LATTICE WITH TOPOLOGICAL DEFFECTS

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We do a mean field analysis for a tight-binding model of electrons hopping in the honeycomb lattice in the presence of first nearest neighbour repulsion. We study a phase transition, of the charge density wave (CDW) type, in which the system undergoes a polarization of the sublattices, above a critical value for the interaction parameter.

The introduction of a topological deffect, by removing a 120º wedge (corresponding to a square at the apex of a cone), is shown to induce a characteristic increase of a local order parameter, equivalent to the polarization of the sublattices within an unit cell, in the vicinity of the defect. The origin of this behaviour may be traced back to a high density of states around the defect near the Fermi level.

We also study the phase diagram when we include a second nearest neighbour repulsion, which leads to topological phases at mean field level, such as a quantum anomalous Hall (QAH) phase, or a Kekulé type phase.

The next step is to analyze the effect of introducing the defect on the phase diagram of our model.

B2 - TOPOLOGY AND DISORDER IN QUADRATIC BAND CROSSING SYSTEMS

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Topological quantum matter has attracted a great deal of attention recently due to the robustness (topological protection) of certain material properties to perturbations like small disorder. As disorder is increased, a topological transition may occur. Here we investigate the interplay between the Chern insulator instability and a local random potential in a model hosting quadratic band crossing points in the clean limit. We determined the phase diagram, figure 1, in the plane of topological mass versus disorder strength, characterizing the system with respect to spectral, localization, and topological properties. In the clean limit, the Chern insulator is characterized by Chern numbers C=+2 or C=-2. Increasing the disorder, the system undergoes a topological phase transition to a Chern insulator with C=+1 or C=-1, absent in the clean limit. A careful analysis shows that these C=+/-1 phases are an instability of the QBCP, appearing for any infinitesimal amount of disorder. These phases occupy a considerable region of the phase diagram for intermediate disorder and show features of topological Anderson insulators: it is possible to reach them through disorder-driven transitions from trivial phases. However, contrary to common topological Anderson insulators, the C=+/-1 phases cannot be explained through a perturbative self-consistent Born approach.

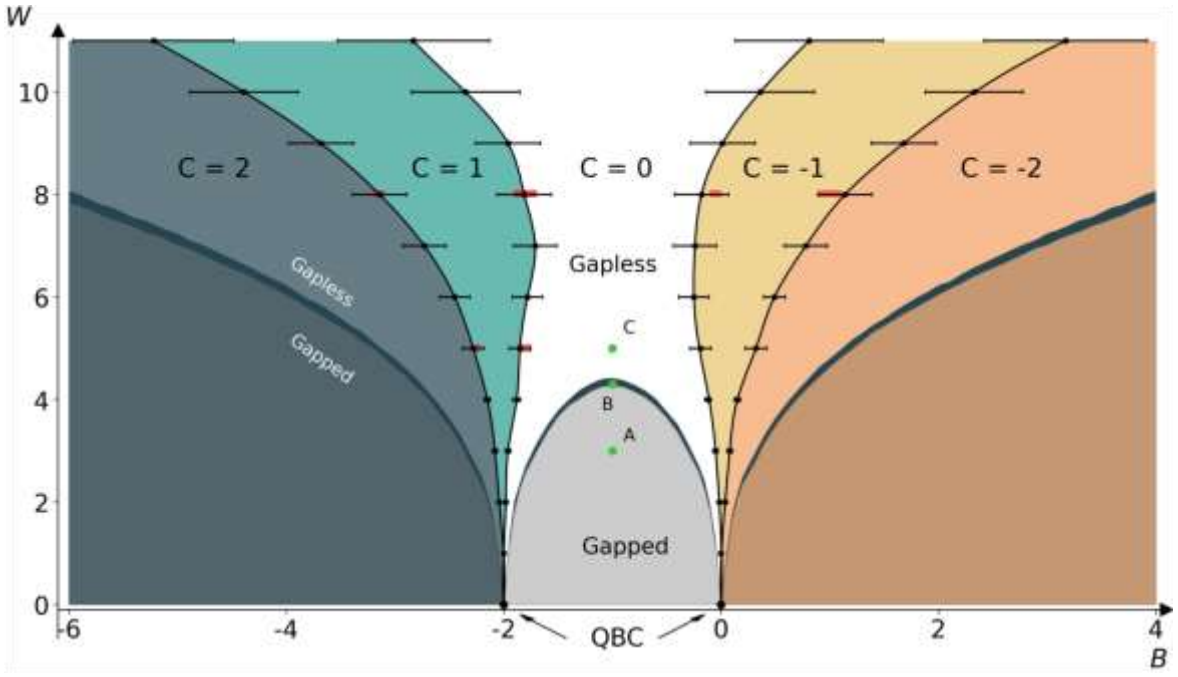

Figure 1: Phase Diagram in the topological mass vs. disorder plane. The colored phases correspond to the different topological phases. The darker blue line correspond to the gapgapless transition.

B3 - EFFECT OF GALLIUM DOPING ON STRUCTURAL AND TRANSPORT PROPERTIES OF THE TOPOLOGICAL INSULATOR Bi2Se3 BY MOLECULAR BEAM EPITAXY

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Three-dimensional topological insulators (TIs) are described by massless Dirac surface states and reduced carrier scattering, due to the presence of strong spin-orbit coupling and the time reversal symmetry (TRS). Bi_2Se_3 is one of the most promising TI due to its relatively large bandgap (0.3 eV [1]), which makes it the most suitable to work at room temperature. Recently, this material has been used to design materials exhibiting quantum anomalous Hall effect [1] and topological superconductivity [2], which are keys for the future of quantum computing. These topological properties can be achieved by doping with specific elements, such as Cu or

Sr [2] however, studies with other elements are scarce. Here, we use molecular beam epitaxy (MBE) to grow high-quality single-crystal films of Gallium-doped Bi_2Se_3. The Gallium addition leads to an expansion of the crystal lattice as demonstrated in the redshifts in the xray diffraction (XRD) (Fig.1 a)) and Raman spectrum. Transport properties were analyzed by a Hall effect and weak antilocalization effect (WAL) at low-temperature, and shows that the Ga doping maintains the n-type semiconductor character but increases the bulk concentration from $8.6x10^{18}$ cm^{-3} to $6x10^{19}$ cm^{-3} at low temperature. While doping the material deteriorates the topological channels observed by WAL, two surface states are still observed at low Ga concentrations as in undoped Bi_2Se_3. Since, both the high electron concentration and the expansion of the crystal lattice are also observed in the topological superconductivity in Cu and Sr doped Bi_2Se_3 [2] it indicates that similar properties could be found in Ga-doped Bi_2Se_3.

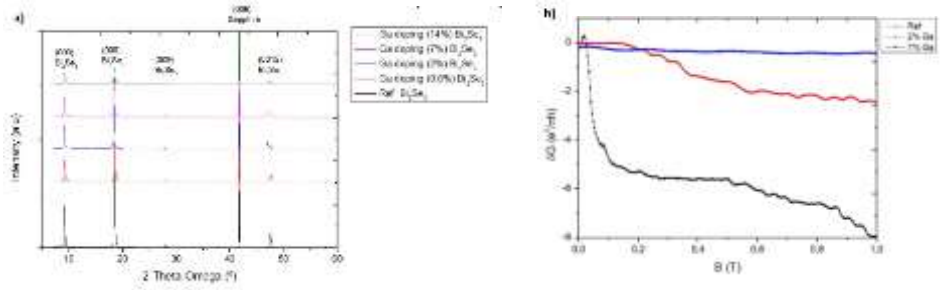

Figure 1 a) XRD spectra of Bi_2Se_3 for different Ga doping. b) WAL magnetoconductance for different Ga doping

Acknowledgments

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B4 - THE HALDANE MODEL IN AN INCOMMENSURATE POTENTIAL

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The Haldane model is a prototypical topological Chern insulator describing electrons in a twodimensional honeycomb lattice with broken time reversal symmetry. The effect of breaking the lattice translational invariance through a disordered, randomly generated potential has been previously studied: the topological robustness to low levels of disorder does not hold at higher levels, and a topological transition to a trivial insulator occurs with increasing disorder strength [1]. On both sides of the transition, the system is an Anderson insulator with finite spectral weight at the Fermi level, becoming a critical metal right at the topological transition. Neither correlated disorder [2] nor unbalanced disorder over the two sublattices [3] change this sate o affairs. Here, we consider the case where translational invariance is broken by applying a periodic hexagonal potential with characteristic lattice spacing that is incommensurable with that of the Haldane model. We show that, similarly to the disordered case, a critical potential strength exists above which the system becomes trivial. This can be seen in Figure 1, where the topological invariant changes from 1 to 0 as the potential *V* increases, signalling the topological transition. Also, in this case a finite spectral weight at the Fermi level accompanies the transition. However, at odds with the disordered case, the localization properties are much less clear and will be discussed.

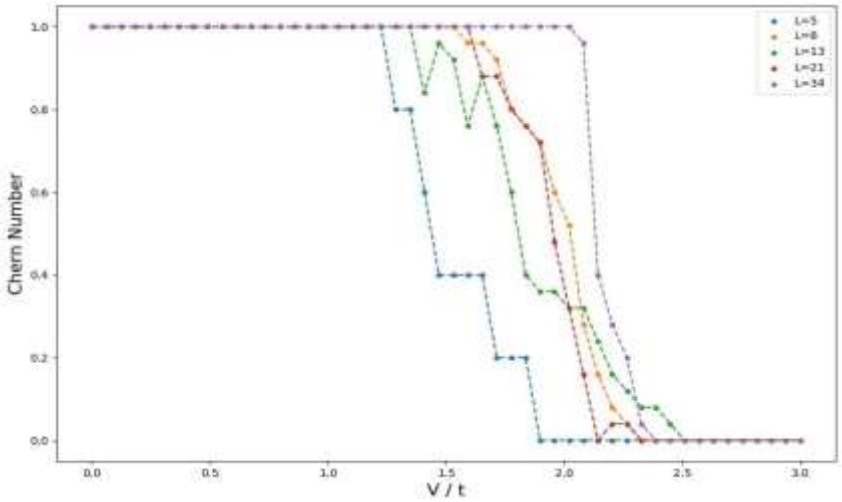

Figure 1. Chern number as a function of incommensurate potential strength.

Acknowledgements

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B5 - DETECTION OF PHASE TRANSITIONS THROUGH AUTOENCODERS

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Recent developments in the field of artificial intelligence (AI), in projects like AlphaGo or GPT3, showed how artificial intelligence can be successfully used to tackle problems that lie outside the conventional mathematical/theoretical framework used to understand reality. Extending these tools to the realm of physics could prove useful in understanding, if not quantitatively, at least qualitatively, models which are analytically intractable even in perturbation theory. One such class of problems, in which these AI algorithms could prove invaluable is the detection of phase transitions.

In this work, we reproduce the results of a previous work [1], in which the phase transition in the two-dimensional Ising model was detected through the analysis of the last layers of a Convolutional Neural Network. Moreover, we also show that the methodology used was not robust enough to enable generalisations to more complex models. Additionally, we also pivot our work in assessing the possibility of improving the previous usage by employing autoencoder arquitectures. It has been proposed [2] that autoencoders [3] can be successfully used to aid the search of phase transitions. Due to their topology, it is reasonable to expect that qualitative changes in the thermodynamic properties of the model will reflect on qualitative changes in the latent variable. We have shown that there is a previously unaccounted bias with respect to the choice of the loss function of the autoencoder and we develop ways to circumvent this, with the introduction of a new architecture: the biphasic autoencoder.

Acknowledgements

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B6 - Detecting phase transitions in- and out-of-equilibrium via single-particle covariance matrices

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In this work we address the problem of detecting phase transitions without prior knowledge of a suitable order parameter. To this end, we propose a notion of metric based on the distance between single-particle covariance matrices. Unlike the well-known fidelity susceptibility, this quantity is accessible to commonly employed numerical techniques and can potentially serve as a versatile instrument to identify phase transitions beyond Landau's paradigm.

In particular, we demonstrate that one choice of metric, which we dubbed single-particle affinity and that coincides with the fidelity for quadratic models can identify non-equilibrium phase transitions. This is shown for a boundary-driven fermion chain under Markovian dissipation, that escapes Landau's framework. We also apply this method to a fermion ladder and find a rather rich phase diagram, contrary to what would be expected from preceding related work on spin ladders.

Acknowledgements

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P. Ribeiro acknowledges support by FCT through Grant No. UID/CTM/04540/2019.

S. Kirchner acknowledges support by the National Key R&D Program of the MOST of China, Grant No. 2016YFA0300202 and the National Science Foundation of China, Grant No. 11774307.

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B7 - Group Theory Analysis to Study Phase Transitions of $Sr_3Hf_2O_7$

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We present an ab-initio study performed by means of Density Functional Theory, groupsubgroup symmetry analysis and lattice dynamics to probe the properties of the octahedral distortions, which occur during the structural phase transitions. Specifically, we focus our study on the $Sr_3Hf_2O_7$ system, which is characterized by a high-temperature *I4/mmm* (S.G. 139) centrosymmetric structure and a ground-state $Cmc2_1$ (S.G. 36) ferroelectric system. We have probed potential candidate phases that may form the I4/mmm → $Cmc2_1$ transition pathways, namely *Fmm2* (S.G. 42), *Ccce* (S.G.68), *Cmca* (S.G. 64) and *Cmcm* (S.G. 63). We found that the band gap widths increase as the symmetry of the systems decreases, with the ground-state structure presenting the largest gap width (~5.95 eV). By probing the Partial Density of States, we observe a direct relation regarding the tilts and rotations of the O perovskite cages as the transition occurs; these show large variations mostly of the O *p*-states which contribute mostly to the valence band maximum. Moreover, by observing the hyperfine parameters, namely the Electric Field Gradients and asymmetric parameters, these vary as the transition occurs, and where the potential phase identification is demonstrated. We have also computed the macroscopic polarization and confirm that the $Cmc2_1$ phase is ferroelectric with a value of spontaneous polarization of 0.0478 C/m^2. The ferroelectricity of the ground-state $Cmc2_1$ system arises due to a second order parameter related to the coupling of the rotation and tilts of the O perovskite cages together with the Sr displacements.

Acknowledgements

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Infrastructure resources, which are partially funded from the European Union's Horizon 2020 research and innovation programme through the ICEI project under the grant agreement No. 800858 and the cluster resources provided by CERN (HTCondor).

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B8 - PRESSURE-INDUCED PHASE TRANSFORMATIONS OF $Sr_3Hf_2O_7$

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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 $Sr_3Hf_2O_7$ compound. Such a system is characterized by a high-temperature *I4/mmm* (space group n. 139) centro-symmetric structure and a ground-state $Cmc2_1$ (space group n. 36) ferroelectric phase. We have probed potential candidate polymorphs that may form the *I4/mmm* towards the $Cmc2_1$ 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. $Ca_3Mn_2O_7$ [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): Γ- and Y-points.

As a continuation of the work done so far in $Sr_3Hf_2O_7$, we apply an external perturbation to study, from a theoretical perspective, the possibility of stabilizing the respective *Ccce* phase at room conditions. Pressure is an important thermodynamic variable which enables the understanding of the properties of materials, even at room pressure, since it allows for a precise control over the interatomic distances and hence the atomic interactions. We will hence show in this work the variation of the structural, vibrational and electronic properties of the *Ccce* structure as a function of applied hydrostatic pressure.

Acknowledgements

This research was supported by the project NECL under NORTE-01-0145-FEDER-022096, Projects CCO 30420916, POCI-01-0145-FEDER-029454, POCI-01-0145-FEDER-032527 and CERN/FIS-PAR/0005/2017. The authors acknowledge computing resources from GRID@FEUP and Advanced Computing Projects (FCT/CPCA/2020/01), CPCA/A2/7087/2020.

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B9 - TRANSITION STATISTICS OF ACTIVE PARTICLES IN TWO-LEVEL SYSTEMS

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The motility of cells is highly influenced by the surrounding environment, posing a theoretical challenge with important applications in the study of cancer and tissue engineering [1,2]. A recent experimental study shows that cells when strong confined in a two-state system can exhibit complex non-linear dynamics, with non-trivial transition rules [3]. Here, we propose an active Brownian particle model to simulate the dynamics of cells when confined in a two-state system composed by two boxes connected by a tunnel. We study how the transition probability between the two boxes is affected by geometric and dynamic properties, such as the length of the tunnel, the propulsion speed, and rotational diffusion coefficient. We show that this rather simple model reproduces the relevant phenomenon observed experimentally.

Acknowledgements

Work with financial support 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, UIDP/00618/2020, and 2020.08525.BD.

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B10 -PHASE STRUCTURE OF THE U(1) LATTICE GAUGE THEORY

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We explore the phases of the compact U(1) gauge theory for different values of the gauge coupling and different numbers of points in the direction of the compactified Euclidean time dimension, Nt. We find that the theory has two phases: a confined phase at strong coupling and a deconfined one at weak coupling. We further calculate the average plaquette, the average Polyakov loop, and respective susceptibilities using lattices with anisotropic spacings, thus determining the value of the critical gauge coupling at which the phase transition occurs for different temperatures and retrieving the phase diagram of the theory.

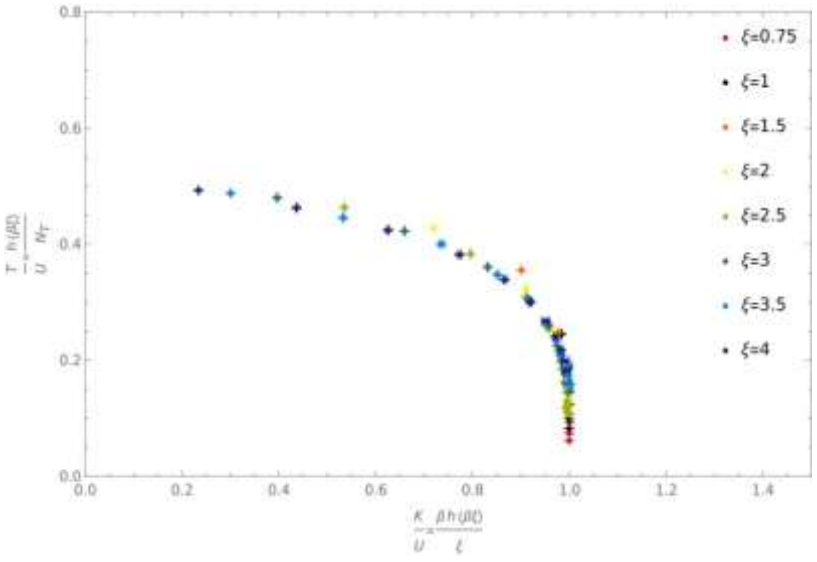

Figure 1. Phase diagram of the U(1) lattice gauge theory in terms of the parameters of the Hamiltonian model.

B11 -CHIRAL DISORDER EFFECTS IN NODAL LOOP SEMIMETALS

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Topological quantum matter has attracted a great deal of attention recently due to the robustness (topological protection) of certain material properties to perturbations like small disorder. Here we investigate the fate of a novel topological system - the nodal loop semimetal - under increasing chiral disorder. Based on a tight-binding model for the nodal loop semimetal where disorder is easily incorporated [1], we developed numerical tools to compute the total winding number of the system. We show that the 3D nodal loop semimetal undergoes a topological phase transition at finite disorder strength, where the topological semimetal gives way to a trivial metal. In Figure 1, the total winding number as a function of chiral disorder strength, for disorder along the direction perpendicular to the nodal loop, is presented. A finite total winding number exists only below a critical disorder strength, signalling the topological phase transition as disorder is increased. Moreover, a re-entrant behaviour where the total winding number increases with increasing disorder is apparent. This indicates that not only the nodal loop semimetal is robust to moderate disorder, it may even become more stable as disorder increases, before the topological transition takes place.

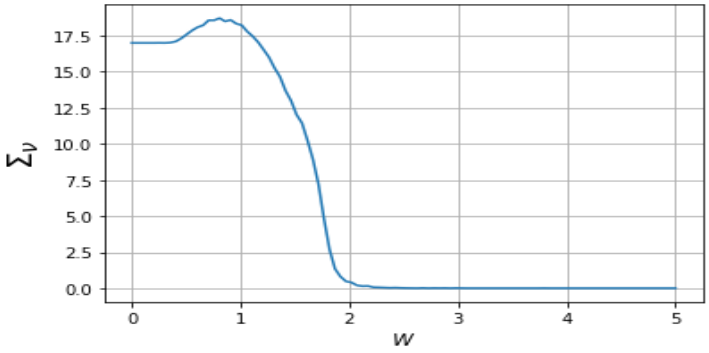

Figure 1: Total winding number as a function of the disorder strength, averaged over 200 disorder configurations. These results were obtained for a system with 100 unit-cells in the direction perpendicular to the nodal loop and 10 × 10 in the directions parallel to the nodal loop.

Acknowledgements

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B12 -SIMULATING MESOSCOPIC TRANSPORT ON FINITE SYSTEMS WITH SPACE-MODULATING HOPPING

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Single-electron states have a unitary time-evolution in the absence of interactions, which imply a finite recursion time to its initial quantum state, provided the Hilbert space is finite. In contrast, in an electrically biased 1D sample sandwiched between two semi-infinite leads, the electrons are naturally driven towards a state of dynamical equilibrium, in which a stationary particle current traverses the sample with a value given by the Landauer-Büttiker formula. This quantum equilibration is made possible by the infinite size of the entire system (leads+sample), and was shown to have an asymptotic Markovian character, with the independent electrons losing memory of the many-particle state in which they were initially prepared. In particular, the stationary state does not depend on the system starting from a partitioned setup [1], where boundary hoppings and different chemical potentials in the leads drive the time-evolution, or a partition-free one [2] where time evolution is generated by the applied bias itself.

Recently, some of us have analysed how this Markovian time-evolution emerges in a disordered tight-binding system with finite "leads", as their size gets larger [3]. While a convergence towards the aforementioned results was verified by increasing the leads' size, several new finite-size effects were unveiled and shown to be controlled by the Fermi velocity inside the leads alone. In this work, we extend the previous study by numerically simulating a similar setup with finite leads that feature hopping strengths that slowly decrease away from the mesoscopic sample. If done smoothly [4], this alteration is expected to slowly modulate the Fermi velocity and speed-up the convergence towards the limit of semi-infinite leads without changing the current that flows through the central sample. For this contribution, we present some preliminary results on quantum transport studied in the simple one-dimensional tight-binding chain. Such a study is a sandbox to create new and more controlled methods for real-space simulations of coherent mesoscopic transport in higher-dimensional setups based upon O(N) spectral expansions with hermitian hamiltonians [4].

Acknowledgements

Work supported by FCT (Portugal) through the Strategic Funding No. UIDB/04650/2020, Projects No. POCI-01-0145-FEDER-028887 (J.P.S.P., S.M.J. and J.M.V.P.L) and the PhD Grants No. PD/BD/142774/2018 (J.P.S.P.) and PD/BD/142798/2018 (S.M.J).

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FRACTAL QUASI-CONDENSATION IN ONE-DIMENSIONAL SYSTEMS

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We study the static properties of one-dimensional quasi-periodic hard-core bosons, using numerically exact methods. A mapping into non-interacting fermionic models is employed, including to the Aubry-André (AA) model and to a generalization of the latter, made by Ganeshan-Pixley-Sarma (GPS model),[1] where anomalous mobility edges - transitions between critical and localized phases - take place.[2] It was previously shown that when the chemical potential is placed in a spectral region of delocalized (localized) fermionic single-particle states, the bosonic system is a quasi-condensate (insulator).[3] We extend this analysis to regimes where the chemical potential lies on critically delocalized states of the fermionic system, unveiling that a novel mechanism for quasi-condensation, here dubbed fractal quasi-condensation, occurs for the hard-core bosons.

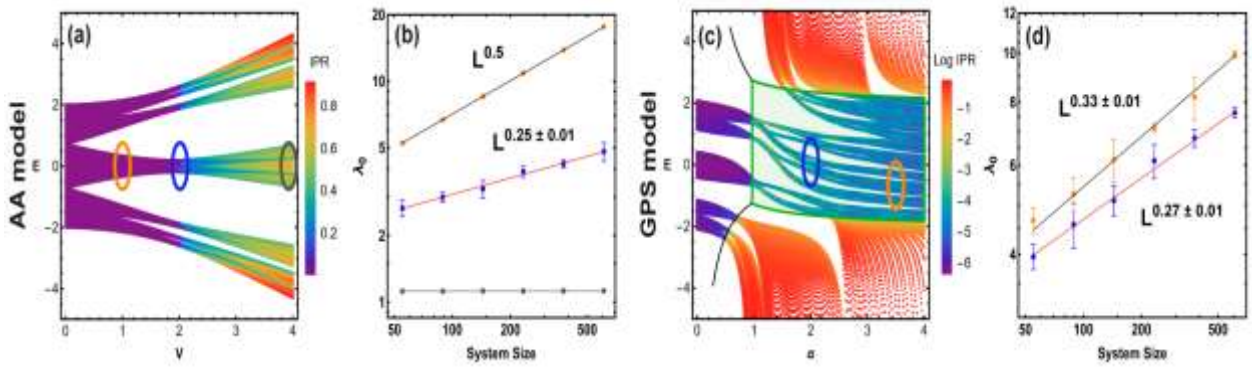

Fig.1 **AA model.** (a) Density plot of the IPR as a function of the single-particle energy (E) and the on-site potential (V), for a system size of L=610. (b) Scaling of the natural orbitals's highest eigenvalue (λ_0) at half-filling (ν=0.5) and V=2 (blue points). Scaling of localized and delocalized states plotted for comparison. **GPS model**. (c) Density plot of the IPR as a function of E and the on-site parameter α, for L=610, V=0.75. (d) Scaling of λ_0 at (ν,α)=(0.48, 2) and (0.368, 3.5), depicted by blue and orange points.

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B13 -SUPERCONDUCTIVITY IN TWISTED BILAYER MIELKE-LIKE SYSTEMS

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Unconventional superconductivity recently observed in twisted bilayer graphene is associated with the presence of two van-Hove singularities very close to the Fermi level reflecting the flattening of two bands for a set of magic twist angles.

In this work, we address a stack of two identical quasi-1D layers, each one composed by a set of chains with p-wave orbitals at each site. When the layers are stacked with a 90º relative angle, the bilayer system resembles the Mielke lattice (which admits one exact flat-band in the one-body tight-binding model for particular values of the hopping parameters).

When a small rotation is applied to one of the layers, regions with different layer stacking appear, and the system, for sizes smaller or of the order of the Moiré pattern unit cell, can be qualitatively described as a n-band model, where each band is associated to a particular region of the lattice. We study the role of these different regions on the superconducting state and in particular on the upper critical field transition curve.

B14 -BLOCH OSCILLATIONS IN DISORDERED WANNIER-STARK LATTICES

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Cold electrons in crystals can have their quantum nature unveiled as an oscillatory behaviour driven by uniform fields. Oscillating currents are well-known to appear as steady-state transport regimes of electrons that move across periodic lattices in the presence of static electric fields [1]. Previous work has further demonstrated this oscillatory behaviour to be present in the propagation of single-electron (gaussian) wave-packets in one-dimensional tight-binding models biased by a sufficiently strong potential ramp. For well isolated bands, the wavepacket's motion is oscillatory and gets confined to a region around the starting position of its center. As the initial gaussian state gets narrowed in real-space, its time-evolution transitions from a coherent sinusoidal oscillation (Bloch oscillations) to an oscillating, but spatially dispersed one (a breathing mode). In both cases the oscillating frequency is proportional to the electric field strength. In contrast, if the system has nearby bands that can be coupled by the potential ramp, through a spectral gap, the effects of Bloch-Zener tunnelling [4] lead to an altered regime of Bloch oscillations that now develop two π-shifted periodic components. In this work, the aforementioned results are re-analysed by numerically propagating the electron wave-packets in real-space using a Chebyshev method [5]. We perform a systematic analysis of a single-band, as well as a gapped two-band (ABAB-lattice) tight-binding model, in which a preliminary study of the robustness of the Bloch oscillation regimes to onsite disordered potentials will be done. The emergence of an oscillating current in tight binding samples, of one and two dimensions, coupled to finite leads with open boundaries is also analysed, and its connection to a ballistic transport regime is drawn via introduction of disorder.

Acknowledgements

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B15 -DIFFUSIVE OPERATOR SPREADING FOR RANDOM UNITARY FREE FERMION CIRCUITS

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Inspired by results on the spreading of operators in generic quantum systems using random quantum circuits [1], in Ref. [2] we study a model of free fermions on a chain with dynamics generated by random unitary gates acting on nearest neighbour bonds and present an exact calculation of time-ordered and out-of-time-ordered correlators. We consider three distinct cases: the random circuit with spatio-temporal disorder (i) with and (ii) without particle number conservation and (iii) the particle non-conserving case with purely temporal disorder.

In all three cases, temporal disorder causes diffusive operator spreading and $\sim\sqrt{t}$ entanglement growth. This is in sharp contrast to Anderson localization for the case of static disorder and with the ballistic behaviour observed in both the clean case of Hamiltonian evolution and in fully random unitary quantum circuits.

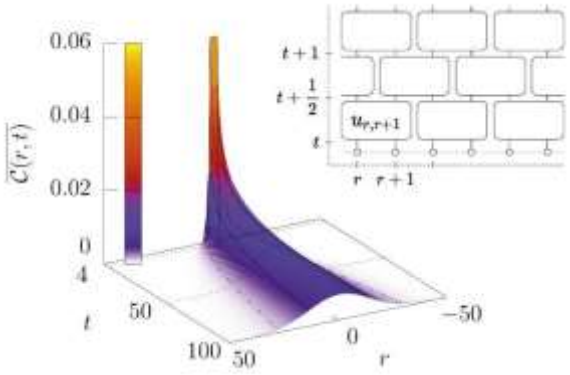

Figure 1. Diffusive spreading of initially localized operators as measured by the correlator $\overline{\mathcal{C}(\bar{r},\bar{t})}$, in a free fermion chain evolved with the random quantum circuit shown as a scheme.

Acknowledgements

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B16 - MOTION OF CHIRAL SWIMMERS IN CROWDED ENVIRONMENT; A STUDY OF THE EFFECT OF NOISE ON THE DYNAMICS

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In this work the dynamics of a chiral swimmer in a crowded environment of impenetrable obstacles is investigated. The obstacles are placed in a regular configuration; different densities of obstacles as fraction of the surface area are considered. The diffusivity of a chiral swimmer is found to be strongly non-monotonic for increasing obstacle density and to display a peak for intermediate densities, when the distance in between obstacles is comparable to the orbit radius of the swimmer. A second less pronounced peak is observed for high obstacle densities, when the distance between the obstacles is comparable to the swimmers size. The first peak is attributed to scattering of the swimmer by the obstacles, perturbing swimming orbits and promoting diffusion. For the second peak, the swimmer is found to be guided by the obstacles. Two types of noise are introduced, noise in the dynamics of the swimmer and quenched noise in the positions of the obstacles. We find that quenched noise can enhance the diffusivity of a swimmer in the presence of obstacles, by preempting fixed swimming orbits, and can suppress diffusivity by limiting the effect of guided motion. Noise in the dynamics enhances the diffusivity for high and low obstacle densities by perturbing swimming orbits and guided motion, but has limited effect for intermediate obstacle densities. Moreover, we find that the increase of noise in the dynamics leads to an enhanced diffusivity. The presence of obstacles can lead to increased and reduced diffusivity for small noise amplitude, but always results in enhanced diffusivity for intermediate noise amplitude and always results in reduced diffusivity for large noise amplitude.

Acknowledgements

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We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under Contracts no. PTDC/FIS-MAC/28146/2017 (LISBOA-01-0145FEDER-028146), UIDB/00618/2020, and UIDP/00618/2020.

B17 -COMBINING EXPERIMENTS AND IN SILICO MODELLING TO INFER THE ROLE OF ADHESION AND PROLIFERATION ON THE COLLECTIVE DYNAMICS OF CELLS

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The collective dynamics of cells on surfaces poses theoretical challenges with important applications in the study of morphogenesis, tissue engineering and cancer [1]. Different mechanisms are at play, including cell-cell adhesion, cell motility and proliferation. However, the relative importance of each is elusive [2]. We developed a particle-based model, which can be combined with experimental results to infer the rate of each mechanism [3]. *In vitro* experiments were performed using a culture of glioblastoma multiform (GBM) cell line, U87MG. The position of the cell nucleus was determined automatically with image processing algorithms and the time evolution of the spatial cell-cell correlation analyzed over a period of 24 h. By parametrizing the adhesion and proliferation rates in the model, it was possible to reproduce the evolution of the two-dimensional spatial heterogeneous distribution of cells, which provides insight into the underlying dynamics. The results revealed a reduction in cell-cell adhesion in response to the increase of cell density in the substrate as a function of time. This mechanism is consistent with a reduction in the contact inhibition and, consequently, an increase enhancement on cells' migration.

Acknowledgements

The authors acknowledge financial support 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. F.R.M. also acknowledges FCT for her contract under the Transitional Rule DL 57/2016 (CTTI-57/18-I3BS(5)).

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B18 -THEORY OF ARPES VISIBILITY IN 2D MATERIALS

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Angle-resolved photoemission spectroscopy (ARPES) allows to probe the electronic band structure of a given crystalline solid. Very often, however, there is a weak or even inexistent experimental signal where band structure theory predicts energy levels to occur. This affects the comparison between theory and experiment, and impairs model validation. Building on the previous work of one of us [1], we have developed computational tools to predict the visibility of different energy bands in an ARPES experiment. The method relies on tight-binding models of the electrons, ensuring its computational efficiency. The differences between theoretical bands and observed ARPES-mapped bands are already made manifest in a toy model diatomic chain. Moving from that, we have applied our approach to several 2D materials: boron nitride and graphene, bilayer graphene (Bernal stacking) [2], and Molybdenum disulfide (MoS2) [3]. The results, of which an example can be seen in Figure 1, show that the visibility of each band depends, not only on the crystal momentum and on the relative phases of eigenstate components, but also on the photon momentum perpendicular to the plane of the 2D solid.

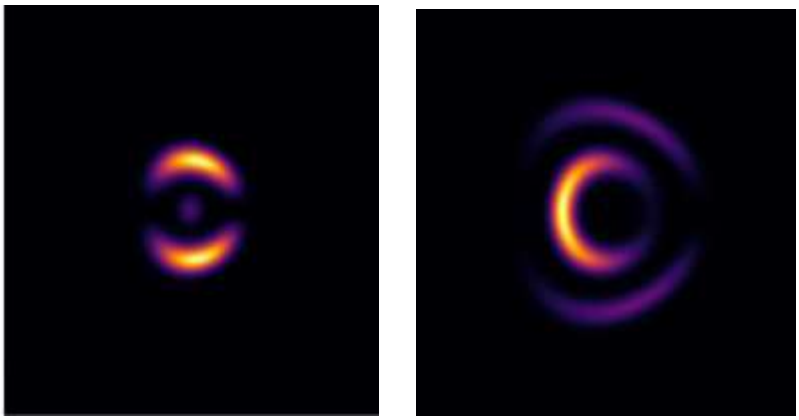

Figure 1. Energy bands visibility for bilayer graphene at energies ε = - 0.2 eV and ε = - 0.5 eV, respectively.

Acknowledgements

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B19 -OPTOELECTRONIC CHARACTERIZATION OF CRYSTALLINE INTERFACES

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Organic semiconductors have unique optical, mechanical, and electronic properties and in the crystalline form they provide an ideal platform for the studies of its intrinsic properties and of the important factors for high performance devices, as they present long-range periodic order and superior features for optoelectronic devices [1]. In order to understand the operation of the excitonic devices, and to allow an improved control of its intrinsic properties, we conducted a study on the behaviour of organic semiconducting single crystals (OSSC), in particular the influence of organic interfaces. Therefore, we have fabricated samples and photonic devices composed of single crystals and crystalline interfaces of remarkable organic semiconductors, such as rubrene, that present long-range exciton diffusion lengths (several micrometers), and absorption in the visible spectral range. The crystals were grown by physical vapor transport and the samples/devices fabricated using lamination and a wire bonding process. Different samples were submitted to photoluminescence and ultrafast transient absorption spectroscopy (Figure 1) and its corresponding devices subjected to optoelectronic characterization. During this study we witnessed an increase of the OSSC device's responsivity (photoresponse) of ~3200% when added another semiconducting crystalline layer, meaning the use of the appropriate organic interfaces could enhance the photoelectric conversion process efficiency of the excitonic devices.

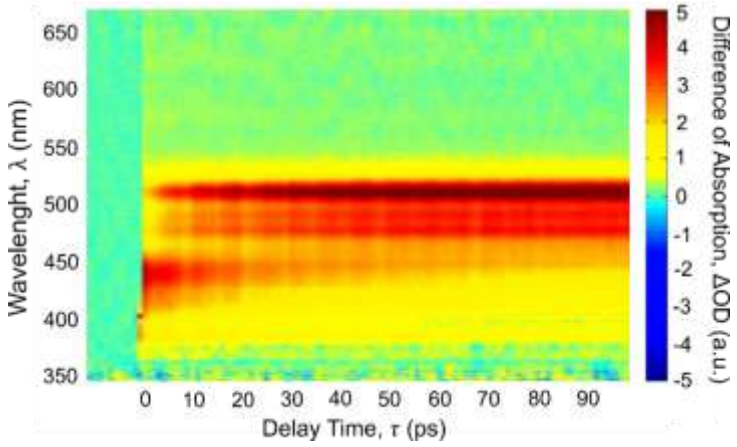

Figure 2. Ultrafast transient absorption spectrum, showing the absorption peaks and the lifetime of the corresponding transitions that occur in an organic crystalline interface sample containing rubrene.

Acknowledgements

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B20 -MAPPING ORGANIC PRINTED FILMS WITH RAMAN SPECTROSCOPY

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Organic crystalline materials are spreading in the optoelectronic field in applications as diverse as field effect transistors [1], photovoltaic solar cells [2] and resistance memories [3]. The most common growth method for these materials has been physical vapor transport [4]. However, for seamless device integration and scalability purposes, printing methods combined with surface energy engineering are currently being explored [5]. In this work, the structural properties of TIPS-pentacene and Rubrene printed films were evaluated using Raman spectroscopy mapping. Figure 1 shows representative Raman spectra along a TIPS-pentacene printed film. The detected narrow peaks are solely attributed to TIPS-pentacene structural fingertip. This work will address the use of microRaman spectroscopy as a powerful tool to map the spatial variation of vibrational modes on organic micrometric printed films.

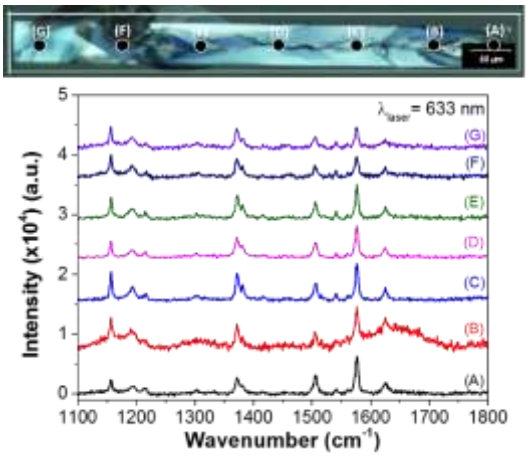

Figure 1. Raman spectra of TIPS-pentacene printed film (50 x 625 μm^2) at positions A to G.

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B21 -PHOTOGALVANIC EFFECTS WITH ULTRAFAST LASER PULSES

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We study the emergence of novel photogalvanic effects (PGEs) excited by ultrashort laser pulses.

A tight-binding model is perturbed by an external electric field, introduced in the system using the velocity gauge [1, 2]. We integrate numerically the Bloch equations for all points in the First Brillouin Zone using a sophisticated parallelized adaptive mesh refinement scheme, capable of distributing computational effort by importance, reducing the time of the overall computation.

We discuss the perturbative and non-perturbative regime and the interplay of the three time scales of the problem – frequency of the pulse, its duration and the scattering duration [3].

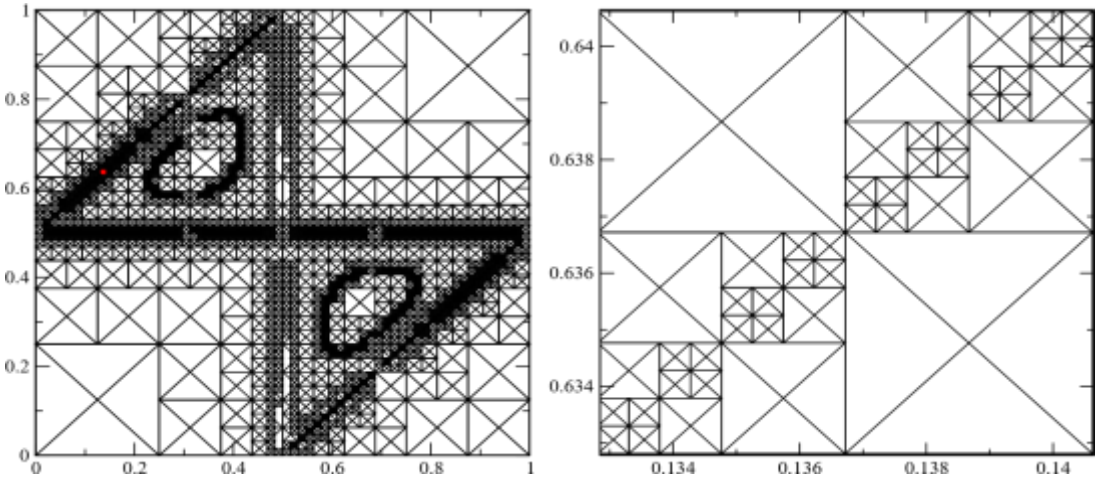

Figure 1. Example of the adaptive scheme for the k-space integration. The right hand side represents an amplification of the red region signalized on the left.

Acknowledgements

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B22 -GIVING SHAPE TO FLEXIBLE MAGNETORESISTIVE SENSORS

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The ability to provide conformable and shapeable devices has opened new doors in wearable technologies and biomedical sensors [1], energy harvesting [2] and photovoltaics [3]. In some cases, the microstructures are required to change their shape and return to their initial state while retaining their properties [4], other applications demand geometrical shapes to be retained while enclosing the working devices [5]. In this work we optimized the shaping of micropatterned magnetoresistive structures using thermal molding. Polyimide and PET foils were used as substrates for the fabrication of the flexible devices, composed of specular spin-valve sensors [e.g., polymer/ buffer/ MnIr/ CoFe/ nano-oxide layer/ CoFe/ Cu/ CoFe/ nano-oxide layer/ free-layer/ cap] and electrical leads. These were patterned using a combination of photolithography, ion milling etching and lift-off steps. Depending on the underlying substrate, different patterning conditions were necessary to achieve well-defined structures. To minimize device failure upon molding, the neutral axis was placed as close as possible to the microstructures' plane [6]. A dedicated protocol was implemented for encapsulation considering SU-8 and polyimide thick layers, compatible with used samples. Thermal molding was then performed using pre-defined cylindrical copper casts. We will discuss the optimization of the molding procedure to achieve the maximum yield of working devices. Electrical and magneto transport measurements of the case studies – specular spin-valves and electrical leads - prior and upon molding will support the analysis and help design the next steps to be taken to improve this approach.

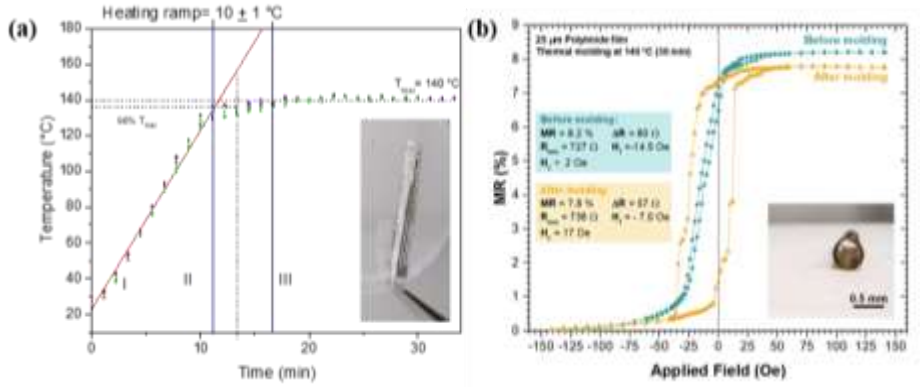

Figure 1. (a) Representative curve for the optimized thermal molding procedure for PET substrates (inset). (b) Example of the output of a micrometric specular spin-valve fabricated on a 25 µm polyimide foil prior and after thermal molding.

Acknowledgements

FCT funding PTDC/NAN-MAT/31688/2017, IF/00713/2015, NORTE/01/0145 /FEDER/22090, UID/05367/2020. FCT grant SFRH/BD/147157/2019. DCL thanks FSE/POPH.

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B23 -LOW IMPEDANCE ELECTRODEPOSITED PEDOT:PSS THIN FILMS

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Introduction: Conductive polymers have been showing great promise in a multitude of areas, especially biomedical applications. In particular, Poly(3,4-ethylenedioxythiophene) (PEDOT) belongs to this family, being one of the most versatile polymers with high electrical conductivity and chemical stability[1], being often doped with poly(4-styrenesulfonate) (PSS) to enable water solubility properties to the copolimer PEDOT:PSS.
PEDOT:PSS has gained attention by researchers due to its thermal, electrochemical and oxidative stability, which allow its applications in flexible electrodes, transitors, solar cells and more. At the same time, its great oxidatative stability enables the use of PEDOT:PSS in biomedical applications. However, the majority of PEDOT:PSS is deposited by spincoating[2], being locked into the manufactures's product preparation with only it's thickness variable. Using electrodeposition combined with simultaneous polymerization, one can make its own custom EDOT:PSS ratios and use the three different possible electrodeposition modes to obtain tunable morphological, electrical and stability properties.
Experimental/Theoretical Study: Three EDOT:PSS solutions where made with 1:1, 1:5 and 1:11 EDOT to PSS concentration. Thin-films deposition of PEDOT:PSS where then performed with a three-electrode setup on Cr/Au substrates. For the electrodeposition process, two different deposition methods were tested: potentionstatic and potentiodynamic. EIS and CV analysis were performed in a three-electrode setup using PBS solution as the electrolyte. Both experiments were performed with a bath temperature of 36ºC. Furthermore, X-Ray Diffrraction, SEM and FTIR were performed, confirming that no contamination was present.
Results and Discussion: To achieve reproducible results, thin film samples of PEDOT:PSS were studied in regards to the deposition parameters/mode and solution concentrations and compared against a similar thickness thin-film of Au. A total of 6 samples (PT 1:1, PT 1:5, PT 1:11, for the potentiostatic mode and PD 1:1, PD 1:5, PD 1:11 for the potentiodynamic mode) were produced. SEM analysis revealed a more porous morphology for potentiodynamic samples, probably arising from the layer-by-layer way in which the deposition of this mode enforces. CV tests, revealed that, overall, all samples had a quasi-square shape indicating a pseudocapacitance nature. Additionally, the potentiostatic samples had a better performance with greater charge storage capacity (CSC), correlated with a larger curve-area, with all PEDOT:PSS samples having much better performance than the Au one (Fig. 1).

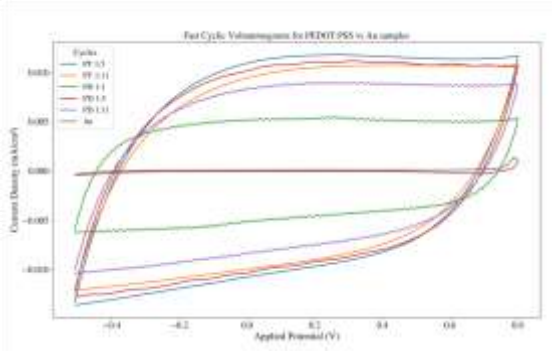

Fig. 1 CV tests performed on all 6 PEDOT:PSS samples and 1 Au sample at 1 V/s

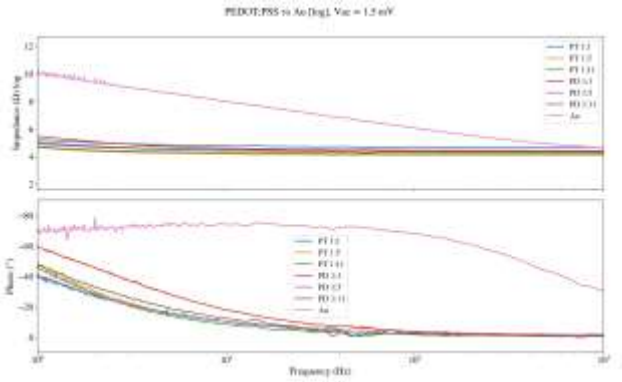

Fig. 2 EIS analysis for PEDOT:PSS and Au samples from 0Hz to 1KHz.

Finally, EIS tests showed that, for 1 kHz, the impedance of the PEDOT:PSS samples were similar. However, the phase of the Au sample was much larger than the PEDOT:PSS. More interestingly, for a lower frequency region (i.e. <1 kHz), the PEDOT:PSS samples impedance is up to 4 times lower, while maintaining a resistive behavior, which is desired for sensitive sensor applications (Fig. 2).

Conclusions: In this work, the impact of different PEDOT to PSS concentrations on the electrodeposition/polymerization of thin-films of PEDOT:PSS was studied, revealing better CSC and impedance response than traditional Au thin-films, making them optimal candidates for various types of sensors.

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The authors acknowledge funding from project PTDC/EMDEMD/31540/2017, POCI-01-0145-FEDER-031540.

B24 -HUMIDITY AND TEMPERATURE TEXTILE SENSOR BASED ON GRAPHENE

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Textile electronics allows the integration of electronic devices in everyday life textile objects. However, it is required advances in materials and manufacturing processes, combining flexibility, electrical properties of semiconductors and metals with solution and low temperature processing [1]. Graphene has suitable properties, such as flexibility, transparency, and high electrical conductivity [2], for textile electronics. Recently, we developed a conductive textile coated with graphene with conductivity of 10^4 S cm^{-1} and sheet resistance lower than 1 kΩ sq^1, maintaining its mechanical properties [3, 4]. We present the development of a dual embedded textile sensor of humidity and temperature based on Few-Layer Graphene (FLG).

The dual sensors are made through coating textiles with a FLG solution, which is done by depositing the solution directly on top of the clean textile samples, through solvent evaporation at controlled temperature. The process does not alter the textile fibers flexibilty and morphology, Fig. 1, adhering to them, and producing a conductive textile. After 1000 bending and 10 washability cycles, the samples maintain their physical and mechanical properties.

The samples were submitted to humidity and temperature tests, in a controlled environment, provided by a climatic chamber. In the range of 10 % to 80 % of relative humidity and 10 ºC to 50 ºC, exists a strong relation between humidity and temperature with electrical conductivity, presenting sensitivity values of $-2.32 \cdot 10^2$ $\%^{-1}$ and $-1.52 \cdot 10^{-1}$ $ºC^{-1}$, 4 and 1 times higher than similar sensors [5]. These results indicate that the dual resistive sensors based on graphene embedded textiles can be used for environmental and biological monitoring applications.

Figure 1. Textile sample: a) before and b) after FLG deposition, SEM image.

Acknowledgements

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B25 - FLUID SIMULATION OF GRAPHENE ELECTRONIC TRANSPORT

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Graphene Field Effect Transistors are excellent candidates for next generation emitters and detectors of coherent radiation in the THz range [1]. Looking to investigate the feasibility and behaviour of these devices, we present a computer simulation [2] developed to study the collective motion of the electrons in graphene in the hydrodynamic regime. Beyond allowing for the application of the boundary conditions to study the Dyakunov-Shur instability, which is explored to excite the graphene plasmons in the inviscid limit, the code can also study the influence of viscosity of an external magnetic field [3]. We focus on the former and particularly on the boundary layer problem and stream velocity profile, as this allows us to better understand the typical dimensions of the system for which viscous effects are non negligible. We found that for sufficiently wide channels the stream velocity profile is no longer parabolic and instead displays a non monotonic profile (Fig.1).

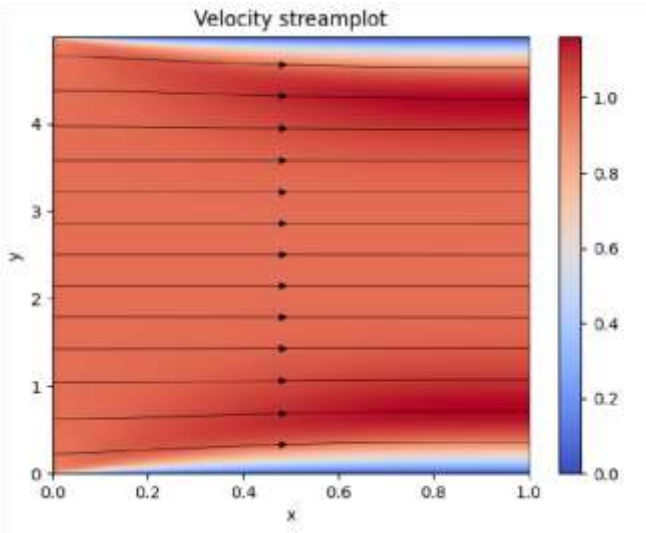

Figure 1: Stream velocity profile for system with $v_x(x = 0) = 1$

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B26 -NONLINEAR DENSITY WAVES IN GRAPHENE'S ELECTRON FLUID

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In graphene, where the electron-electron scattering is dominant, electrons collectively act as a fluid [1]. This hydrodynamic behaviour of charge carriers leads to exciting nonlinear phenomena such as solitary waves and shocks, among others. In the future, such waves might be exploited on plasmonic devices [2,3] either for modulation or signal propagation along graphene waveguides. We study the nature of nonlinear perturbations by performing the reductive perturbation method [4] on the hydrodynamic description of graphene's electrons [5], taking into consideration the effect of Bohm quantum potential and odd viscosity [6]. Thus, deriving a dissipative Kadomtsev-Petviashvili (KP) equation for the bidimensional flow as well as its unidimensional limit in the form of Korteweg-de Vries-Burgers (KdVB). The stability analysis of these equations unveils the existence of unstable modes (Fig. 1) that can be excited and launched through graphene plasmonic devices.

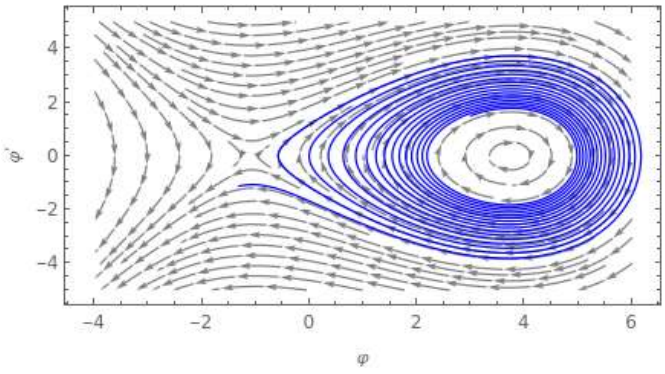

Figure 1. KdVB phase portrait for density evolution highlighting an unstable solution.

Acknowledgements:

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B27 - SEMICLASSICAL APPROXIMATION FOR NON-HERMITIAN OPERATORS – APPLICATION TO STOCHASTIC OPTIMIZATION

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In this work, we study the semiclassical dynamics of non-Hermitian quantum systems in phase space. The non-Hermitian semiclassical dynamics of Gaussian coherent states is described by a system of equations for the motion of the center and of the metric associated with the wave packet, which we call the intrinsic geometry of the state [1,2]. The inclusion of a non-Hermitian part leads to the non-conservation of the norm, which can be interpreted as either energy loss or gain. Analytical and numerical methods of solving the dynamics of non-Hermitian quantum systems in phase space are studied and developed. Lastly, a connection is made between the formalism of stochastic optimization of a certain class of control systems and the semiclassical evolution generated by a quantum non-Hermitian Hamiltonian. An example of a quadratic Hamiltonian is explored where we show the existence of the infinite time limit of the center and the metric of the wave packet.

Acknowledgements

We thank the financial support provided via the project (1801P.00819.1.01) GASonSQuaTPTDC/MAT-OUT/28784/2017 and also via the project UIDB/04459/2020 from FCT.

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SYNCHRONIZATION OF OSCILLATORS IN A FLUID

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Particles moving in a fluid interact though flows leading to rich non-linear behaviors. A problem of interest is the synchronization in biological flows at the microscale, such as the synchronization of bacteria flagella and the transport of organelles in living organisms by cilia. In this work, we used the lattice Boltzmann method to simulate moving solid particles in a fluid and simulate the fluid-particles interaction. First, we validated our method by calculating the drag force of a moving cylinder at constant velocity in a fluid. Next, we study the influence of an oscillating particle in a second one which was initially stationary as a function of the distance between them, viscosity and frequency of oscillation. We also investigate the coupling between two oscillators in a fluid.

Acknowledgements

We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under the contracts no. UIDB/00618/2020 and UIDP/00618/2020.

B28 -FIRST-PRINCIPLES MODELLING OF THE PHASE STABILITY AND SEGREGATION OF HYDROGEN AT THE ABSORBER-BUFFER INTERFACE IN CHALCOPYRITE-BASED SOLAR CELLS

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Understanding the impact of impurities and dopants in solar-cell $CuInSe_2$ chalcopyrite absorbers remains a challenging problem that has been addressed by both theoretical and experimental studies. Hydrogen, in particular, can be frequently found in thin-film solar cells, either incorporated from the surrounding environment during film growth or through various annealing treatments alongside the film deposition. In a typical cell the front part is composed of the heterojunction which is formed between the $CuInSe_2$ absorber and a buffer material (usually chosen to be CdS). This part receives the sunlight which in turn creates electron and hole carriers. The present study reports calculations based on density-functional theory that examine the behaviour of hydrogen in the bulk-crystalline $CuInSe_2$ phases and the $CuInSe_2$/CdS heterojunction. The latter has been modelled by two distinct faceted interfaces by joining the respective chalcopyrite and zinc-blende (CdS) lattices through their common polar {112} crystallographic planes. The calculations provide essential information on the electrical levels of hydrogen in bulk $CuInSe_2$ and the type of configurations that hydrogen impurities can form locally at the core of the interfacial facets. The results are also discussed in the light of recent experimental observations by various solid-state spectroscopies.

Acknowledgements

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B29 -STRUCTURAL EFFECTS ON BIOFILMS OF ACTIVE PARTICLES OF DIFFERENT LENGTHS

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Active particles belong to a class of non-equilibrium systems with a persistent local entropy production, which violates detailed balance. This gives rise to a novel type of collective behavior such as the coexistence of vapor- and liquid-like steady states for active particles with repulsive interactions only. Similar to bacteria, active particles tend to accumulate at confining surfaces forming dense adsorbed films [1].

In this work, we aim to study how active particles accumulate near a surface according to their size. Furthermore, we want to know the evolution of their collective behavior focusing mainly on analyzing the influence the particle length has on the created biofilm. We performed Langevin dynamics simulations and studied two different cases: ellipsoids and rods (Figure 1). We observed a biofilm spreading along the wall for near spherical shape and a tendency to form drops when particles are elongated.

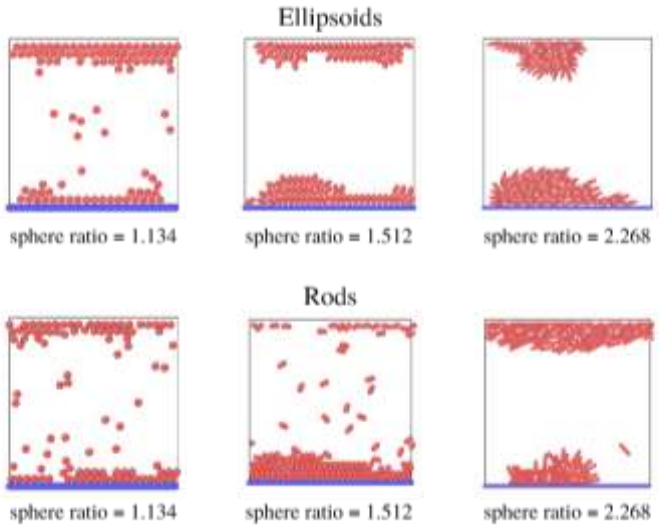

Figure 1. Snapshots of the evolution of particle agglomeration. Top the results for ellipsoids and bottom results for rods.

Acknowledgements

We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under Contracts no. PTDC/FIS-MAC/5689/2020, CEECIND/00586/2017.

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B30 -VALIDITY OF THE ENVIRONMENT-ASSISTED QUANTUM TRANSPORT IN DIFFERENT LIGHT-HARVESTING SETTINGS

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The exciton transport in photosynthesis has been raising a lot of interest by the research community after the unexpected observation of its coherence across light-harvesting molecules in photosynthesis by 2D electronic spectroscopy experiments [1]. One of the possible causes of the high efficiency of this transport probably is the exciton interaction with the environment, termed as *environment-assisted quantum transport* (*ENAQT*) [2,3]. The environment plays a crucial role at enhancing the efficiency of the exciton transport by introducing a moderate degree of dephasing in the electronic molecular degrees of freedom. In this work, we show that the efficiency of the exciton transport can be controlled not only by the dephasing rate introduced by the environment (ENAQT), but also by the rate of the exciton-extracting process, which in photosynthetic systems is equivalent to the *Förster Resonance Exciton Transfer* (FRET) rate from the lightharvesting system to the reaction center. This is demonstrated by phenomenological simulations of the dissipative Lindblad equation applied to the exciton transport (see Figure 1 for a description of the model). This work aims at understanding whether the ENAQT regime may explain the high efficiency of the photosynthetic exciton transport in different light-harvesting settings.

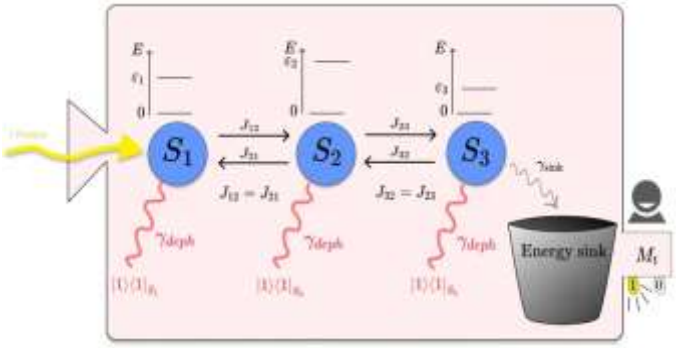

Figure 1. Exciton transport across a chain of three light-harvesting molecules, S_1, S_2, S_3 and the energy sink. J_{ij} denotes the electromagnetic coupling between the molecules *i* and *j* and the energy diagrams above them show the chosen site energy for each molecule, modelled as a qubit. The Markovian environment, illustrated as the pink box surrounding the molecules, interacts with the molecule *i* with a constant rate γ_{deph} via the Lindblad operator $|1\rangle\langle 1|_{Si}$. The energy sink, represented by a qubit, receives the energy dissipated from the last molecule in the chain to the sink with an extraction rate γ_{sink}. Lastly, we choose the observable M_t to be the projection operator $|1\rangle\langle 1|$ applied to the energy sink qubit at time *t*.

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B31 -AIRFLOW-DRIVEN HYBRIDIZED NANOGENERATOR FOR BIOMECHANICAL ENERGY HARVESTING

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Introduction

The increasing use of wearable electronics, such as fitness trackers, calls for sustainable energy solutions. These electronic devices are normally powered by batteries [1], which need to be replaced every so often due to their limited lifespan. This leads to the disposal of millions of batteries every year, increasing environmental pollution. Biomechanical energy harvesting appears as a potential solution to this problem, as the human body generates a significant amount of power during gait motion, sufficient to drive small electronics [2]. Triboelectric nanogenerators (TENGs), a recent technology based on the triboelectric effect [3], emerge as the most promising approach due to their light weight and high power density at low frequencies [4].

In this work, a TENG was hybridized with an electromagnetic generator (EMG) to harvest energy from the foot strike during gait motion. A small and enclosed radial-flow turbine, actuated by a pair of air bulb pumps placed on the shoe insole, was used to convert the foot-strike linear movement into rotational motion of the hybridized nanogenerator.

Methods

We designed and optimized the proposed turbine using two different software: *SOLIDWORKS 2020* (computer-aided design) and *Ansys 2021 R1 CFX* (computational fluid dynamics). The optimized models were then 3D printed from polylactic acid and tested using an experimental setup which included a pneumatic motor to compress the air pumps. The tribomaterials consisted of a FEP film and an organic textile operating in the freestanding mode.

Based on this design, we placed the TENG laterally, with the FEP film attached to one of the rotor blades, and the organic textile and Cu electrodes fixed on the stator inner-side wall. The EMG consisted of four disk-shaped NdFeB magnets attached directly to the rotor topside, with the Cu coils fixed above. Finally, the whole prototype was integrated into a commercial shoe to power small electronics from foot pressing.

Conclusions

In summary, a hybridized triboelectric-electromagnetic nanogenerator was developed to harvest energy from the foot-strike induced airflow. The turbine mechanism enhanced the motion frequency by a factor over 10, which resulted in an output power above 240 μW. The hybridization between TENG and EMG improved the charging of a capacitor compared to each individual generator, which was then used to power small commercial electronics.

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B32 - FLEXIBLE TRIBOELECTRIC NANOGENERATORS FOR A SELFCHARGING SYSTEM IN MOBILE ELECTRONICS

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A rapid development in personal electronics has raised challenging requirements for their portable and sustainable power sources. For example, in wearable technologies, the concept of wearable body area network (WBAN) brings body motion and vital signs monitoring together in synergy [1]. For this, a key aspect is sustainable portable energy, available anywhere, at any time, as generated by triboelectric nanogenerators (TENG) for flexible and efficient self-charging systems. This technology usually demands high-cost processes and materials and still suffer from low power output, as well as unstable output values due to charge generating stimulus with variable intensities. In this work, we present TENGs using graphene as electrodes as well as active triboelectric layer deposited by a simple solution process. In addition to graphene, other low-cost materials such as conventional polymers were used taking advantage of solution processing methods as spin coating, and screen-printing. Different device structures are also explored to optimize performance depending in the tribo-response. Device electrical power generation was tested with a stable physical stimulus for better understanding of the working mechanism. TENGs based on the triboelectric response of PDMS vs graphene showed open circuit voltages reaching few hundreds of volts and short circuit currents of tens of nano amperes when stimulated at 1.5Hz. A power density of 5.85 μW/cm^2 under a load of 1GΩ (figure 1) was achieved. These results demonstrate the potential of solution process for low-cost triboelectric devices for wearable flexible nanogenerators.

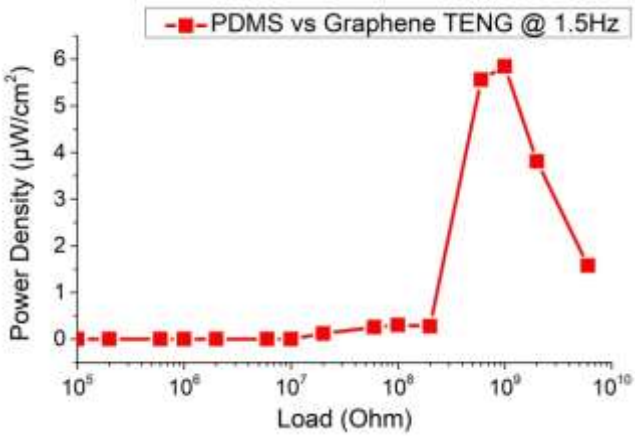

Figure 1. Output power density of TENG based on the triboelectric response of graphene/PDMS with various load resistances.

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B33 - ALL *IN-SITU* STUDY OF IONIC LIQUID GATING ON OXIDES

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Ionic liquid gating has been shown to provide a promising way to control the electronic properties of materials, for example, to induce metal to insulator transitions. When used as gate dielectric in a field effect transistor structure, ionic liquids allow charge transfers up to 2 orders of magnitude larger (at lower gate voltages) when compared to common solid-state dielectrics. For many materials, however, the mechanism behind the charge carrier doping has been shown to be not purely electrostatic. Instead, electrochemical mechanisms have also to be considered. Yet, which electrochemical processes are actually taking place are still under discussion. In most studies reported in the literature so far, the samples or the liquids are exposed to air at some point in the experiment, such as during the device fabrication or the ionic liquid injection. Since ionic liquids are hygroscopic, exposure to air may lead to contamination, changing the properties of the liquid by reducing its electrochemical window. This may be the reason for the lack of consensus within the community. Thus, a study performed all under ultra-high vacuum conditions is required to ensure that there is no contamination of the sample or the liquid. Here we present an all *in-situ* study of ionic liquid gating on different oxide materials (Fe_3O_4, TiO_2, $SrTiO_3$ and EuO_{1-x}) which includes the sample and device preparation, injection of the liquid and the gating measurements.

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B34 - SUPERCAPACITORS FOR A WEARABLE ALL-FIBRE DEVICE

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To date power supply of electronic textiles devices has been done by conventional batteries, which besides having low durability, are heavy and difficult to directly integrate into a textile (*e.g.* without stamping). Hence, to fill the gap, we present a project not only aiming at developing discreet, lightweight and durable energy storage devices, directly weaved in a textile, but also aiming at enabling simultaneous solar energy harvesting. As by integrating both technologies into a single device, one can deal with the intermittent nature of solar energy, and provide the long-awaited wearables full-day energy autonomy. All-fibre integrated photovoltaic-storage devices (All-FIBRE device) are being achieved by two different innovative approaches. Both giving origin to functional yarns made with non-flammable and non-toxic materials and making use of simple, fast and inexpensive processes, scalable for mass production in industry. Final devices will allow wet or dry cleaning.

First project results will be presented, focusing on the design and testing of a 1D carbon fibre supercapacitor made in the braid-like configuration [1]. It was made with commercial carbon threads as electrodes and a simulated sweat solution as electrolyte. The goal was evaluating its applicability to sport textiles. The separator and electrolyte container were made with an electrospun cellulose acetate fibre membrane. Nevertheless, an alternative to electrospinning technique has been evaluated by exploring faster newer processes. The carbon treads were functionalized with polypyrrole to enhance surface area and improve specific capacity (0.62 F/g). Cyclic voltammetry and charge-discharge cycling shown device washability and electrochemical stability.

Acknowledgements

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Presenting Authors Index

R

S

T

V