Non-identical moiré twins in bilayer graphene

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The superlattice obtained by aligning a monolayer graphene and boron nitride (BN) inherits from the hexagonal lattice a 60◦ periodicity with the layer alignment. This implies that the mechanical, optical and electronic properties of the heterostructure must be identical for 0◦ and 60◦ of layer alignment. Surprisingly, this periodicity apply only for the monolayer case. In this talk, I will show you that the moiré superlattice formed by a bilayer graphene aligned with BN, is present every 60◦, but the symmetry is broken between the 0◦ and 60◦ alignments, creating non-identical moiré twins with different electronic properties. In particular, electron transport measurements display a fully developed valley Hall effect at 0◦ while it is completely absent at 60◦. The origin of the non-identical moiré twins is explained by studying the relaxation of the atomic structures using state-ot-the-art numerical techniques, which highlight the central role of the Bernal stacking configuration with respect to the BN layer. Our results challenge the current understanding of the valley Hall effect, since a simple Berry curvature argument do not hold to explain this 120◦ periodicity in bilayer graphene/BN. This unique interplay between mechanical and electronic properties, demonstrated by the in situ control of the rotational order, increases the possibilities for band-structure engineering on van der Waals heterostructures.

Piezoelectricity and ferroelectricity in hexagonal boron nitride

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Two-dimensional (2D) hexagonal boron nitride (hBN) is a wide-bandgap van der Waals crystal with a unique combination of properties, including a honeycomb lattice very close to that of graphene, exceptional strength, high oxidation resistance at high temperatures and optical functionalities [1]. As a result, it has become a ubiquitous material for the fabrication of van der Waals heterostructures [2]. Like many Group III nitride materials, its covalent bonds are highly polar, presenting the possibility of piezoelectric and spontaneous polarizations in the correct crystal configurations. In this talk, I first describe the observation of in-plane piezoelectricity for monolayer (one atom thick) hBN [3], a property that does not exist for bilayer or bulk systems. Next, I report the occurrence of spontaneous out-of-plane polarization and ferroelectricity at anomalously stacked hBN interfaces [4]. We have observed these effects using atomic force microscopy (AFM) electrical modes, namely electrostatic (EFM) and Kelvin Probe (KPFM) Force Microscopy, in combination with detailed modelling of in-plane deformation profiles and interface relaxation. Both the in-plane piezoelectricity and out-of-plane ferroelectricity presented here open up interesting possibilities for precise control of device properties. The experimental approach used here also shows a way to investigate the polarization properties of other materials at the nanoscale.

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Figures

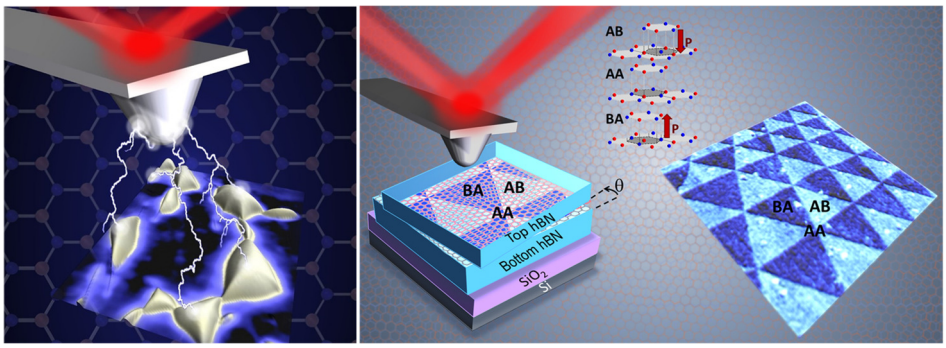

Figure 1: Piezoelectricity and ferroelectricity in hBN.

Magnetic Kondo lattices in two-dimensional transition metal dichalcogenides

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Metallic dichalcogenides like 1T-$TaSe_2$ present an uncommon charge density wave state which produces an array of isolated, unpaired electrons that form a lattice of magnetic moments. In this talk, I will present both theory and experimental results on the 1T/1H-$TaSe_2$ heterostructure, where the magnetic moments in the T layer are coupled to the Fermi surface of the H layer and form a Kondo lattice. Our STM experiments do reveal a Kondo peak which is however split at very low temperatures. I will then discuss how this splitting and its dependence on magnetic field are not consistent with a Kondo screened, paramagnetic lattice, and rather point to a magnetic ground state with small Kondo exchange. I will then present ab-initio calculations to estimate the Kondo coupling and discuss our results in terms of an Anderson model. Our work uncovers these dichalcogenides as a natural platform to study Kondo lattices [1].

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Figures

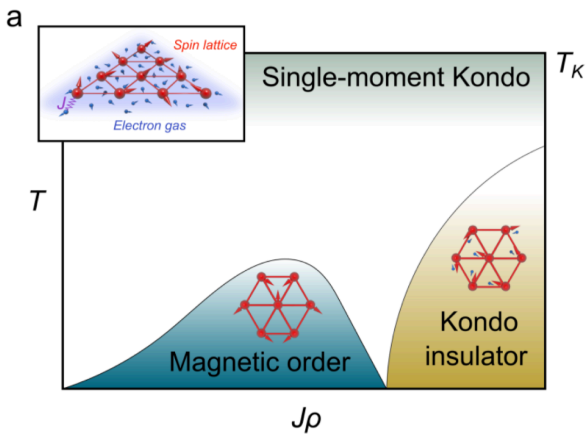

Figure 1: Schematic Doniach diagram showing the competition between magnetic and Kondo screened phases. The inset shows the effective triangular Kondo lattice realized in transition metal dichalcogenide heterostructures.

Universal moiré nematic phase in twisted graphene

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Graphene moiré superlattices display electronic flat bands. At integer fillings of these flat bands, insulating states due to strong electron–electron interactions are generally observed. However, the presence of other correlation-driven phases in twisted graphitic systems at non-integer fillings is unclear. We report [1] the existence of three-fold rotational (C_3) symmetry breaking in twisted double bilayer graphene. Using spectroscopic imaging over large and uniform areas to characterize the direction and degree of C_3 symmetry breaking, we find it to be prominent only at energies corresponding to the flat bands and nearly absent in the remote bands. We demonstrate that the magnitude of the rotational symmetry breaking does not depend on the degree of the heterostrain or the displacement field, being instead a manifestation of an interaction-driven electronic nematic phase. We show that the nematic phase is a primary order that arises from the normal metal state over a wide range of doping away from charge neutrality. Our modelling suggests that the nematic instability is not associated with the local scale of the graphene lattice, but is an emergent phenomenon at the scale of the moiré lattice. This suggest that nematic instabilities are common in moiré systems and may be universal elements of their phase diagrams.

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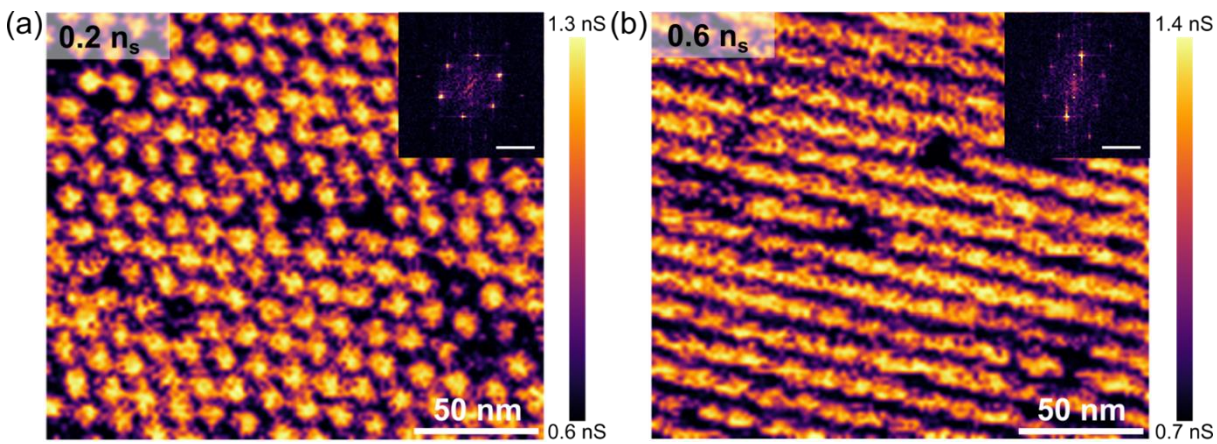

Figure 1: (a), (b), dI/dV maps at the energy of the VFB, close to charge neutrality (a) and around half-filling of the CFB (b). The insets show the fast Fourier transform of each LDOS map.

Graphene field effect transistors for THz technology and applications

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Terahertz (THz) frequency range is still known as one of the least exploited and investigated ranges of the electromagnetic spectrum. Located between the millimeter waves and infrared domain has hazy defined range from about 100 GHz up to 10 THz. THz waves have revealed a great potential for use in various fields and for a wide range of challenging applications such as security, material sensing, future 6G wireless or quantum communication among others. To this aim, high-performance detectors are, vital for exploitation of THz technology. Thus, on the last years, there was a huge scientific interest for the development of new THz devices and techniques. A very special attention has been given to graphene plasmonic THz detectors as they have started to emerge as a promising platform for a new generation of optoelectronic devices, but improving their performance is still necessary. In the lecture we will show how graphene nanostructures forming lateral asymmetric superlattices (Figure 1) can be used for sensitive THz detection operating up to room temperature. Here we will demonstrate that novel approaches and mechanisms could lead to enhance the performance on these graphene-based THz detectors [1]. Furthermore, as a proof of concept two clear examples with these devices will be presented to be used for terahertz sensing of hidden metallic objects at room temperature [2] and as a platform for the experimental observation of the nontrivial topological gap in graphene [3].

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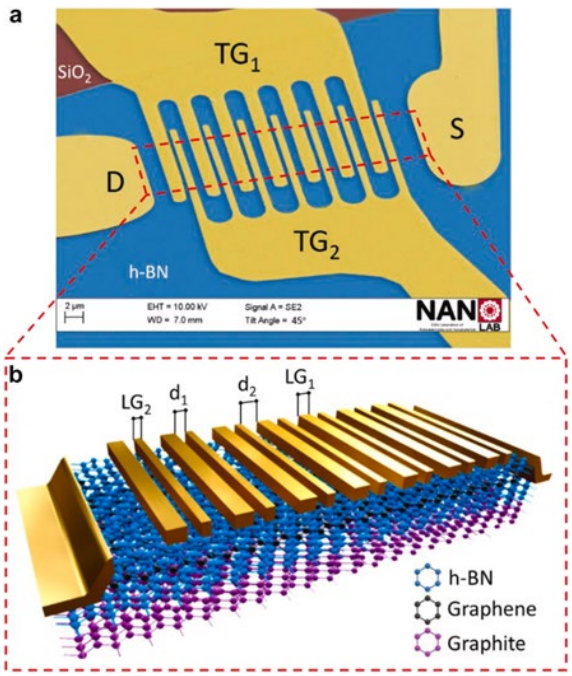

Figure 1: A graphene-based THz detector

Non-reciprocal charge transport in chiral Tellurium nanowires

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Charge-to-spin conversion enables the electrical generation of spin currents without magnets.[1] For instance, the flow of a charge current generates a net spin polarization in materials characterized by strong spin-orbit coupling and broken inversion symmetry through the Edelstein effect. Lacking inversion and mirror symmetry, chiral materials such as elemental Te (Figure 1a) are the ideal playground to explore the relation between structural symmetry and electronic spin transport.[2] Here, we report a chirality-dependent and gate-tuneable charge to spin conversion in single-crystalline Te nanowires.[3] The generation of a net spin polarization is inferred by recording a dependence of the nanowire resistance on the relative orientation between electrical current and applied magnetic field (Figure 1b,c). By analyzing this non-reciprocal charge transport, we show that an electrical current generates a spin polarization oriented along to the chiral axis and pointing in opposite direction for different crystal handedness. Theoretical calculations indicate that this charge-to-spin conversion arises from the radial spin texture of the valence band of Te. In addition, the electric field generated by a gate electrode modulates the amplitude of the non-reciprocal charge transport by a factor six, indicating the possibility to electrically manipulate the efficiency of the charge-to-spin conversion. The all-electrical generation, control, and detection of spin polarization in chiral Te nanowires opens the path to exploit chirality in spintronic devices.

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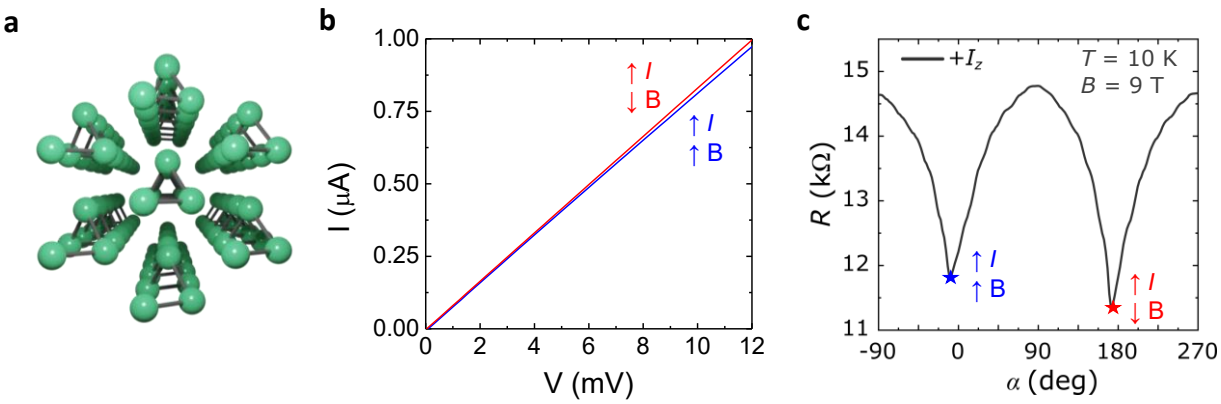

Figure 1: a. 3D sketch of the Te crystal structure. **b.** Different current-voltage traces are recorded when the magnetic field is applied parallel or antiparallel to the current, corresponding to different resistance. **c.** Resistance of a Te nanowire as a function of the angle α between the current direction and an external magnetic field.

Non-perturbative indirect exchange in spin-valley coupled 2D crystals

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In this work[1], we study indirect exchange interactions between localized spins of magnetic impurities in spin-valley coupled systems described with the Kane-Mele model. The model captures the main ingredients of the energy bands of 1H transition metal dichalcogenides (TMD) monolayers. These systems present anisotropic interactions that include Heisenberg, Ising and Dzyaloshinskii-Moriya couplings. In contrast to previous studies [2-4], we calculate the indirect exchange by using exact diagonalization of the Hamiltonian, avoiding the use of perturbation theory and the momentum cut-off. We study the interplay between the symmetry of indirect exchange (Heisenberg, Ising and DM), the Fermi-surface topology and the relative orientation between the magnetic impurities. We find that the anisotropic nature of the interaction depends on the impurities orientation. Moreover, we relate the contribution of intervalley or intravalley electronic scattering processes with the Fermi-surface topology. We also test the validity of the perturbative results and conclude that it is a good approximation beyond the expected regime. Finally, we show that the effective Hamiltonian derived from perturbation theory works in the non-perturbative regime.

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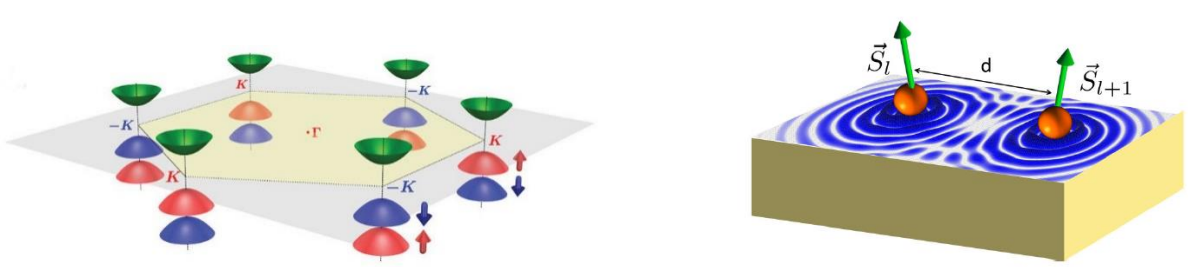

(a) (b)

Figure 1: (a) Schematic drawing of the spin-valley coupled band structure (Picture taken from [5]). (b) Scheme of the mechanism of the indirect exchange interaction between two localized surface spins (Taken from [6])

Universality of moiré physics in collapsed chiral carbon nanotubes

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The discovery of superconducting and correlated insulating behavior in twisted bilayer graphene (TBG) has shaken up the field of two-dimensional (2D) materials, reinvigorating the study of graphene-based systems. We demonstrate that one-dimensional moiré patterns, analogous to those found in twisted bilayer graphene, can arise in collapsed chiral carbon nanotubes (CNT) [1]. Performing a detailed study of the electronic structure of all types of chiral nanotubes, previously collapsed via molecular dynamics and validated against ab-initio modeling, we find that magic angle physics occurs in all families of collapsed carbon nanotubes [2]. Velocity reduction, flat bands, and localization in AA regions with diminishing moiré angle are revealed. Remarkably, all kinds of nanotubes behave the same with respect to magic angle tuning, showing a monotonic behavior that gives rise to magic angles in full agreement with those of TBG.
Superconductivity in TBG was an unexpected phenomenon, so the quest for other systems which could be the 1D analogues of TBG is of great importance to elucidate the nature of superconductivity found therein. Moreover, nontrivial topological phases have been found in the magic angle regime and are closely related to flat bands. Therefore, chiral collapsed carbon nanotubes stand out as promising candidates to explore topology and superconductivity in low dimensions, emerging as the one-dimensional analogues of twisted bilayer graphene.

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Figures

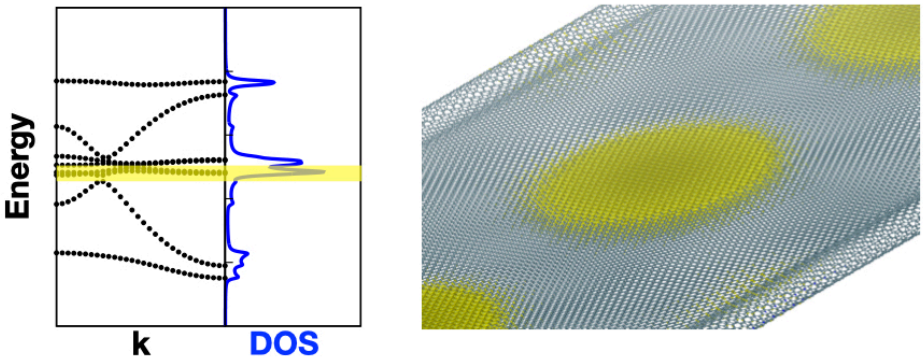

Figure 1: Left panel: Band structure and total DOS for a (164,2) collapsed nanotube. The two highest valence bands are highlighted to indicate the range of energies occupied to map the spatial localization of those states. Right panel: lateral view of the structure with the local DOS of the aforementioned bands highlighted in color. The states are localized in the AA regions of the nanotube unit cell.

When active matter turns solid : from collective motion to collective actuation

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Active matter is made of a large number of out of equilibrium interacting units, which convert some source of energy into directed motion. In contrast with systems driven out of equilibrium by an external field, or through the boundaries, the departure from equilibrium is local and independent for each active unit. Not so surprisingly, active matter exhibits rich collective phenomena at large scales, such as new types of phase separation and/or collective directed motion. The past 25 years have seen a surge of experimental observations and theoretical progress in the description of such phenomena in the realm of active liquids.

There are however a number of circumstances under which the description in terms of liquids is not suited. One can think of ants building solid bridges out of their bodies, meta-materials made of mechanically connected engines, cohesive cell layers or simply very dense assemblies of self propelled particles forming a glass or a crystal. In such cases a description in terms of elastic solid is likely to be more appropriate. However very little is known about the actuation of an elastic lattice by polar active particles, the orientations of which may couple to the displacement field.

In this talk, I will present very recent experimental and theoretical works aiming at developing this new path of research in active matter. Doing so, we shall unveil a new type of collective phenomena, namely collective actuation, and discover how the coupling between linear elasticity and activity leads to a rich selection mechanism of the actuated dynamics.

Rotating vesicles to mimic cell motion

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Cells move through complex media to perform vital biological processes, often following environmental cues. Because the cell membrane is sticky, rather than slipping on surfaces, cells exploit friction to perform controlled motions on surfaces. When two adhering surfaces, the cell membrane and the substrate, are moved across each other, a finite force must be exerted to break the intermolecular bonds across the shearing interface, and these bonds may reform, fully or partially, during sliding. Despite of their importance and complex nature, the tribological properties of cell membranes remain largely unexplored in literature. Therefore, here, we present a minimal cell model to measure and study the tribological properties of cell membranes. The model consists of a vesicle, an aqueous droplet stabilized by an amphiphilic membrane, produced by microfluidics [1], encapsulating a magnetic microparticle in the core, as illustrated in Figure 1. External actuation of the microparticle results in the rotation of the vesicle, which slides on the substrate, enabling tracking of the vesicle motion. Using this approach, we show that rotating vesicles can move exploiting hydrodynamic friction, and that the vesicle velocity can be modified by fine tuning of membrane mechanical properties. Incorporation of protein receptors in the vesicle membrane and specific ligands on the substrate may result in directed motion along gradients in the mechanical properties or ligand concentration in the substrates [2].

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Figures

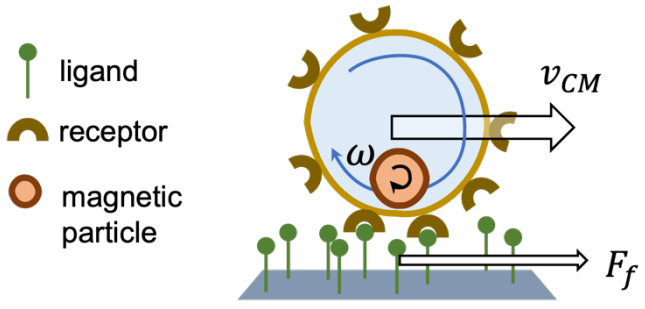

Figure 1: Schematic illustration of a vesicle that rotates upon external actuation of an encapsulated magnetic particle and translates on a substrate with a typical velocity v_{CM} due to a friction force, F_f.

Non-equilibrium active switching of soft colloids: microstructure, phase behaviour and heterogeneous dynamics

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We explore the microstructure and phase behavior of a nonequilibrium system comprised by soft colloids that can actively switch their interactions between two states at a predefined kinetic rate. For this purpose, we employ a Reactive Dynamical Density Functional Theory (R-DDFT) and reactive Brownian-Dynamics simulations (R-BD). We find that the switching rate interpolates between a near-equilibrium binary mixture at low rates and a nonequilibrium monodisperse liquid for large rates, strongly affecting the one-body density profiles, adsorption, and pressure at confining walls. Importantly, we show that sufficiently fast switching impedes the phase separation of an (in equilibrium) unstable liquid, allowing the control of the degree of mixing and condensation and local microstructuring in a cellular confinement by tuning the switching rate [1, 2].
Switching activity also modifies the dynamics and diffusion coefficients of the individual particles, leading to a crossover from short to long times, with a regime for intermediate times showing anomalous diffusion [3]. The corresponding self-intermediate scattering function shows the two-step relaxation patters typically observed in soft materials with heterogeneous dynamics such as glasses and gels. R-DDFT results are in excellent agreement with R-BD simulations and the analytical predictions of a phenomenological Continuous Time Random theory, thus confirming that R-DDFT constitutes a powerful method to investigate not only the structure and phase behavior, but also the dynamical properties of non-equilibrium active switching colloidal suspensions.

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Nematics in solid tori: Doubly twisted structures and defect populated configurations

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Nematic liquid crystals are partially ordered fluids characterized by an apolar vector field, called director, that represents the average orientation of its anisotropic building blocks. Confining a nematic liquid crystal can frustrate its order, leading to the presence of topological defects, which are regions where the alignment is not defined. Each topological defect can be characterized by a quantity called topological charge. Mathematically, the Poincaré-Hopf index theorem relates the total topological charge to the confining topology. For instance, a 2-sphere must have a total topological charge of +2, so that the presence of defects is mathematically required. In the case of a toroidal surface, the total topological charge must be equal to 0, and thus defect free configurations of the material are allowed. In prior experimental work in our group, we filled a solid torus with a nematic liquid crystal and found spontaneous chiral symmetry breaking without defects [1]. In this talk, we will report on alternative defect-populated configurations [2]. These have s=±1 pairs, with the s=+1 and s=-1 defects most often located in regions of positive and negative Gaussian curvature respectively. Remarkably, we also observe these defect pairs in cylinders. The key is the similar free energy of both defect-free and defect-populated configurations separated by a large free energy barrier.

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Lattice resonances: a collective response of periodic arrays of nanostructures

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Periodic arrays of metallic nanostructures are able to support collective modes known as lattice resonances. These excitations occur at wavelengths commensurate with the periodicity of the array and give rise to very strong and spectrally narrow optical responses. Thanks to these exceptional properties, periodic arrays are being exploited in a wide variety of applications, including ultrasensitive biosensing, nanoscale light emission, and color printing, to cite a few.

In this talk, we will discuss some recent theoretical advances on the topic of lattice resonances. We will pay particular attention to the near- and far-field properties of these modes and how they depend on both the characteristics of the array and the source used to excite them.

Temporal and spatiotemporal metamaterials

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In this talk I will first introduce the basic concepts of wave interactions in time varying media. I will discuss how temporal modulations of the electromagnetic parameters offer new pathways in wave control with metamaterials, as energy is not necessarily conserved in these time-dependent systems, and non-reciprocal effects can be realized [1].

Next, I will concentrate on a class of space-time metamaterials where parameters are modulated in a travelling-wave form, such that there is an apparent motion of the optical properties. Through an homogenization theory that provides analytical expressions for the effective permittivity, permeability and magnetoelectric coupling of these media, I will show how non-reciprocity arises even in the quasistatic limit [2] and how the synthetic motion present in these systems allow us to make a link to the Fresnel drag effect of light in moving media [3]. Additionally I will discuss how an unconventional linear gain mechanism takes place when the modulation travels close to the speed of light [4], resulting in nonreciprocal and broadband amplification that could be realised with graphene [5]. Finally, I will present an implementation of an Archimedes screw for light that leads to chirally-selective amplification [6].

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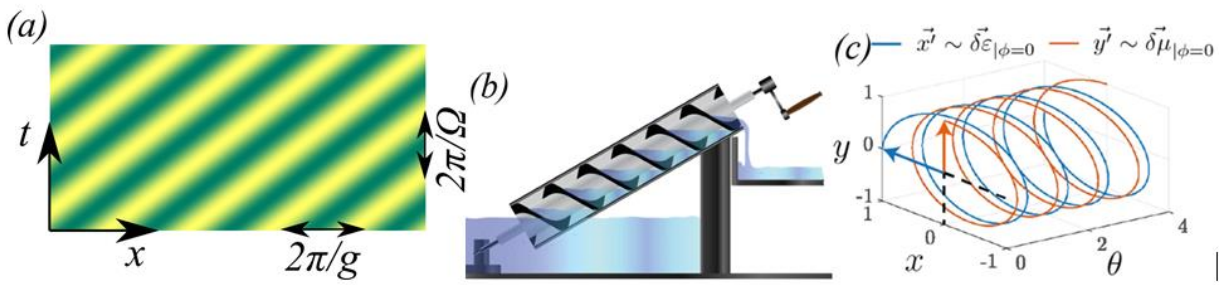

Figure 1: (a) Sketch of pace-time modulation of the permittivity and/or permeability of travelling wave kind. (b) A mechanical Archimedes screw carries fluids from a lower to a higher ground. (c) An optical screw is a medium whose permittivity and permeability tensors are modulated such that the principal axes of their modulation describe two helices in the spatio-temporal coordinate.

Fast response photogating in monolayer MoS_2 phototransistor

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Two-dimensional transition metal dichalcogenide (TMD) phototransistors have been the object of intensive research during the last years due to their potential for photodetection. Photoresponse in these devices is typically caused by a combination of two physical mechanisms [1-2]: the photoconductive effect (PCE) and photogating effect (PGE). In earlier literature for monolayer (1L) MoS_2 phototransistors, PGE is generally attributed to charge trapping by polar molecules adsorbed to the semiconductor channel, giving rise to a very slow photoresponse. Thus, the photoresponse of 1L-MoS_2 phototransistors at high-frequency light modulation is assigned to PCE alone. In this work [4] we investigate the photoresponse of a fully h-BN encapsulated monolayer (1L) MoS_2 phototransistor. In contrast with previous understanding, we identify a rapidly-responding PGE mechanism that becomes the dominant contribution to photoresponse under high-frequency light modulation. Using a theoretical model for the photocarrier dynamics, we fit the illumination power dependence of this PGE and estimate the energy level of the involved traps. The resulting energies are compatible with shallow traps in MoS_2 caused by the presence of sulfur vacancies.

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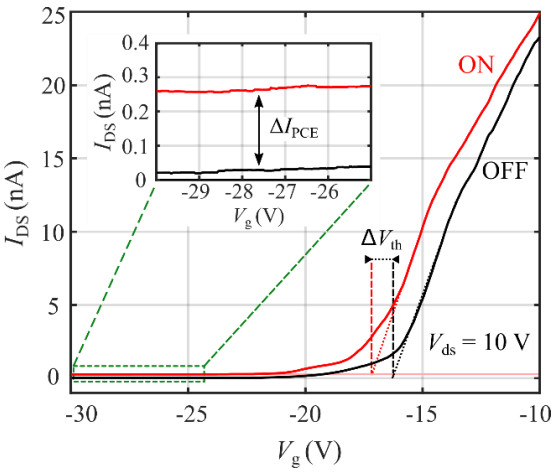

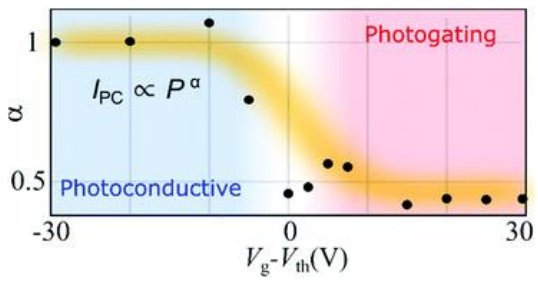

Figure: a) Gate transfer curves of the device, showing a threshold gate voltage V_{th} = −11 V. The inset shows a zoom-in of the region indicated by the dashed green rectangle. The contributions to photoresponse by ΔI_{PCE} and ΔV_{PGE} are indicated in the plot. b) Dependence of the fitting parameter α on V_g−V_{th}. The two different regimes for power dependence are indicated in the figure

Imaging of Anti-ferroelectric Dark Modes in an Inverted Plasmonic Lattice

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Plasmonic lattice nanostructures are of technological interest because of their capacity to manipulate light below the diffraction limit. Here, we present a detailed study of dark and bright modes in the visible and near-infrared energy regime of an inverted plasmonic honeycomb lattice by a combination of state-of-the-art Au+ focused ion beam lithography, optical and electron spectroscopy, and finite-difference time-domain simulations. The lattice consists of slits carved in an Au thin film, exhibiting a plethora of resonances in the visible and near-infrared ranges.
A detailed description of the charge distribution and near-field enhancement has been given by virtue of the good agreement between the electron energy loss spectroscopy (EELS) measurements, the optical measurements, and simulations. The most remarkable result is the finding of dark modes that may be caused by antiferroelectric arrangements of the slit polarizations, giving rise to charge arrangements with a unit cell four times larger than that of the original honeycomb lattice (see Figure 1(b and 1e). Additionally, bright plasmonic modes exhibiting hotspots far from the metal slits are also found. The studied plasmonic resonances take place within 0.5 and 2 eV energy range, indicating that they could be suitable for a synergistic coupling with excitons in 2D transition metal dichalcogenides materials or for designing nanoscale sensing platforms based on near-field enhancement over a metallic surface. For example, the exciton energies for 2D WSe_2 and MoS_2 on an Au substrate, 1.75 and 1.9 eV, respectively [1], could be targeted by easily tuning manufacturing parameters such as the pitch of the lattice, thus changing the spectral position of the plasmonic resonances.

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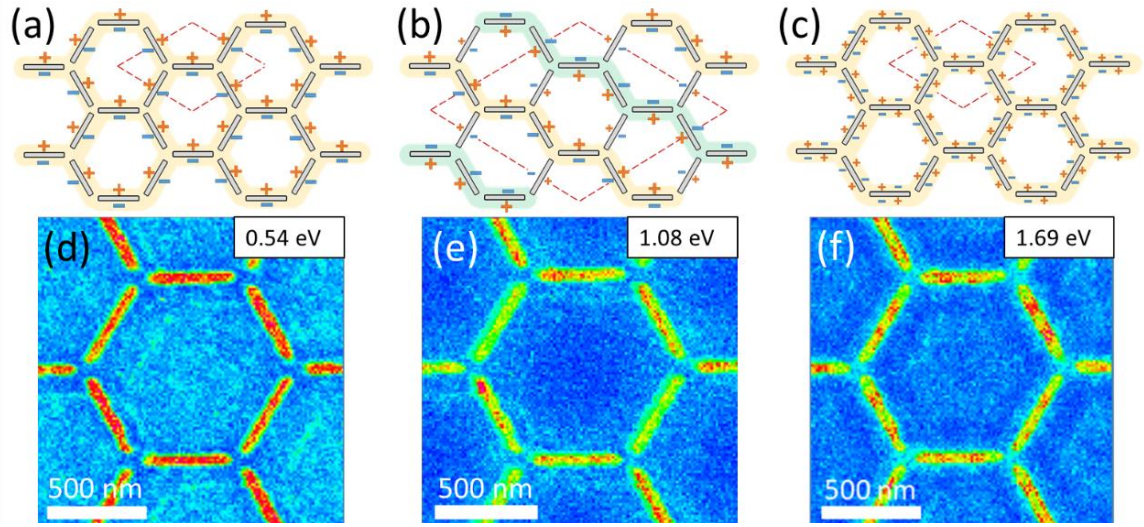

Figure 1. Plasmonic modes measured in the lattice at three different energies. (a), (b) and (c) show schematic representations of the charge distributions associated with one bright and two dark modes, respectively. Panels (d), (e) and (f) present the EELS mapping for the each of the modes depicted in the upper panels.

The emergence research landscape of altermagnetism

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Antiferromagnetic spintronics has been one of the most active research areas of condensed matter in recent years. As we have learned how to manipulate and understand antiferromagnets actively and their emergent topology, further surprises awaited. Turning off spin-orbit coupling, a new fresh view at the family of antiferromagnetic ordered systems reveals also an emergent new class, dubbed altermagnets, with properties unique to itself and separate from ferromagnets and antiferromagnets. We report the discovery of a third distinct magnetic phase, beyond the conventional ferromagnetism and antiferromagnetism, with non-relativistic alternating spin-momentum locking, which we dub "altermagnetism". We show that this new phase is as abundant in nature as conventional ferromagnetism and antiferromagnetism, while it displays properties unparalleled in the two traditional magnetic phases, such as spin splitting by electric crystal field. Remarkably, altermagnetism was missed over the past century of quantum-magnetism research because it cannot be identified by the conventional crystallographic and relativistic magnetic symmetries, established since the early works of Bethe, Landau, Shubnikov and others. This altermagnetic phase emerges naturally when utilizing the spin-symmetry formalism, where spin and real space are decoupled.

Direct X-ray detection of the spin Hall effect in CuBi

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The spin Hall effect, and its inverse, are important spin-charge conversion mechanisms widely investigated due to their fundamental importance in the development of spintronics devices. Their measurement is typically done by electrical detection schemes involving an interface with another magnetic material and thus, a combination of the properties of both materials as well as the interface are measured. The large scattering of reported results from these methods for the same material and temperature call out for a more direct and interface-free approach. Optical detection schemes have been successfully used for the determination of SHE in semiconductors. This approach is, however, challenging for metallic systems, due to their considerably shorter spin diffusion lengths. Only recently, optical measurements for Pt and W have been reported [1].
Considering that x-ray magnetic circular dichroism (XMCD) has become a reference tool for precision measurement of small or diluted magnetic signals, we propose the use of XMCD-PEEM microscopy for direct, interface-free determination of SHE in metals. In particular, we report the observation of spin separation due to SHE in a single layer of Bi-doped Cu (Cu95Bi5), a material in which giant SHE has been reported [2,3]. We performed interface-free x-ray spectroscopy measurements at the Cu L3,2 absorption edges while applying electrical current to the sample. The sign of spin accumulation depends on the direction of the current (Figure 1.a) and the amplitude of the X-ray magnetic circular dichroism (XMCD) signal scales with the current density and has different sign when measuring at the L2 or L3 absorption edges, as expected for SHE (Figure 1.b). We have measured an induced magnetic moment of (2.7 ± 0.5) x 10-12μB A-1 cm2 per Cu atom averaged over the probing depth, which is of the same order as for Pt measured by magneto-optics. Our results constitute the proof of concept for the direct, interface free and element-selective measurement of the SHE in a single material by means of X-ray spectro-microscopy, and highlight the potential of CuBi for spin-charge conversion applications[4].

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All-electrical spin control in low-symmetry materials

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The existence of the quantum spin Hall (QSH) insulator has boosted opportunities for spintronics and quantum metrology, given the ability of topologically protected states to convey spin information over long distances at ultralow dissipation rate. QSH is a manifestation of strong spin-orbit coupling. However, even in time-reversal symmetric systems, the lack of a spin conservation axis in QSH insulators allows backscattering effects for edge states, limiting their ballistic transport. In some situations, the emergence of a phenomenon known as persistent spin texture (PST) enforces spin conservation and favors long spin lifetimes even in the presence chemical disorder and structural imperfections. Such an effect is deeply rooted in the underlying symmetries of the system and opens promising prospects for spintronics when combined with the manifestation of dissipationless chiral edge states. The recent prediction and experimental observations of a PST-driven canted quantum spin Hall effect in low-symmetry monolayer WTe2 provide new ingredient for the use of topological materials in spintronic applications.

This work reports on the possibility of a fully controllable variation of up to 90 degrees rotation of the spin polarization of chiral edge-states, dictating the canted QSH effect, while preserving spin conservation. By combining density functional theory (DFT) with tight-binding methods and quantum transport simulations, we show that the emerging PST can be continuously varied from in-plane to out-of-plane under electric fields below 0.1 V/nm, making this effect experimentally accessible. The experimental confirmation of such fully electrically tunable spin-polarized topological currents would establish a new milestone towards replacing magnetic components in spintronic devices and all-electric spin circuit architectures, as well as optimized resistance quantum standards.

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Coexistence of structural and magnetic phases in van der Waals magnet CrI_3

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Amidst the members of the family of layered materials, chromium triiodide (CrI_3) was the first one to demonstrate the persistence of a ferromagnetic hysteresis down to the monolayer as well as a layer-dependent transition from a ferromagnetic to an antiferromagnetic state [1]. Following this discovery, a plethora of studies appeared providing evidence that the origin of this thickness-dependent magnetism relies in the crystalline stacking order, thus revealing a strong coupling between magnetism and crystal structure [2,3,4]. However, to date, bulk CrI_3 keeps hosting fundamental conundrums such as the emergence of a peak at 50 K in the in-plane magnetization curve, and controversies, such as having a range of temperatures for the crystalline phase transition [4,5]. Combining muon spin rotation, magnetization and low temperature X-ray diffraction measurements (Figure 1) we reveal the emergence of two unexpected magnetic phases as well as the persistence of 10 % of the monoclinic phase at low temperature. These two events give hints of a rich phase diagram regarding 2D magnetism in CrI_3, which goes far beyond the assumed monoclinic/rhombohedral dichotomy.

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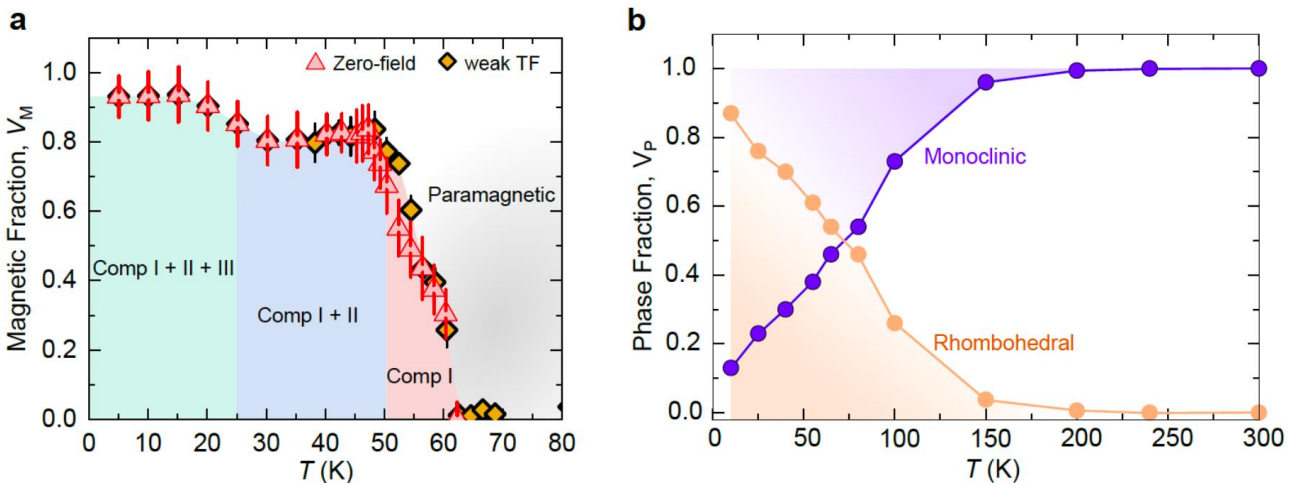

Figure 1: a, Temperature dependence of the total magnetic volume fraction V_M determined by zero field μSR measurements. **b,** Crystalline phase fraction obtained from Rietveld refinements on temperature dependent X-ray diffraction measurements.

Cryogenics for Quantum Technology and Condensed Matter Physics
Oxford Instruments

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Experiments at low temperatures, down to a few milliKelvin and at high magnetic fields offer unique opportunities to probe the physics of quantum materials.
In this presentation, Oxford Instruments NanoScience will share how sophisticated instrumentation allows us to study the fascinating properties of materials - reaching temperatures down to 10 mK and magnetic fields up to 14 Tesla and more!
Find out how the cryofree Proteox and TeslatronPT are creating ultra-low temperature environments under high magnetic fields to unleash materials discovery.

Figure 1: ProteoxMX Dilution Refrigerator

Lightwave Control for Sub-Cycle and Non-Resonant Valley Manipulation in 2D Materials

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Modern light generation technology offers extraordinary capabilities for sculpting light pulses, with full control over individual electric field oscillations within each laser cycle [1]. These capabilities are at the core of lightwave electronics on a few-cycle to sub-cycle timescale, aiming at information processing at peta-Hertz rates. At the same time, quantum materials encompass fascinating properties such as the possibility to harness extra electronic degrees of freedom, e.g., the valley pseudospin, that can be optically initialized via resonant circular pulses [2,3,4]. Still, initializing, manipulating and reading the valley degree of freedom on timescales shorter than valley depolarization remains a crucial challenge.
I will present an all-optical, non-resonant approach to control the injection of carriers into the valleys by controlling the sub-cycle structure of non-resonant driving fields [5]. For triangular sub-lattices, such as those of hexagonal boron nitride (hBN) or MoS2, the bicircular field, formed by a circular field and its counter-rotating second harmonic, possesses the symmetry of the sub-lattice and is shown to initialize a high degree of valley polarization on a sub-cycle timescale. The valley pseudospin is then read by using either the imprint of the Berry curvature on the high harmonic generation spectrum in non-inversion-symmetric monolayers [5] or by quantifying the appearance of even harmonics due to the breaking of inversion symmetry created by the valley polarization [6].

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Figures

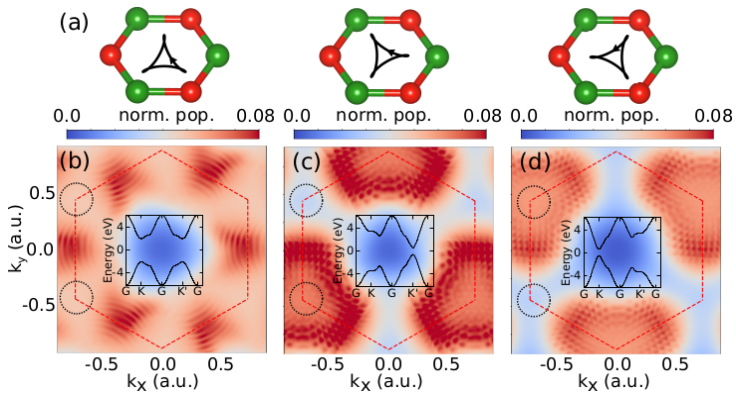

Figure 1: (a) Different orientations of the bicircular field with respect to the lattice, controlled by the phase delay between the two colors. (b-d) Normalized electron population in the lowest conduction band of hBN after applying the bicircular field above with 3 micron of fundamental wavelength.

Optical bistability based on the integration of a molecular nanomaterial in Silicon Photonics

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Electro-optical bistability is a functionality which can be crucial for a wide range of applications as it can enable non-volatile and ultra-low power switching performance [1]. In this work an advance in Nanophotonics is presented with a new approach for the development of low-power on-chip optical switching devices. This new approach is based on the integration of an encapsulated molecular nanomaterial that presents bistable Spin Crossover (SCO) phenomenon near room temperature (RT) in the Si platform [2].
SCO is a spin-state switching phenomenon present in some molecular compounds such as the coordination complexes of transition-metal ions in which, under certain external stimulus (variation of temperature, pressure, electric field, or light irradiation), the electronic configuration can be switched between two molecular spin states, Low Spin (LS) and High Spin (HS) states [3]. Furthermore, the spin state change is accompanied by a change in the structural, magnetic, and optical properties, as well as in the electrical conductivity and color. These properties vary as a function of the external stimulus following a hysteretic response, recognized as one of the most promising aspects of the system since hysteresis confers bistability and thus a memory effect (Figure 1a).
Finally, the SCO material can be synthetized as nanoparticles so that it can be easily integrated in the silicon platform and have the potential to allow optical switching at room temperature (Figure 1b).

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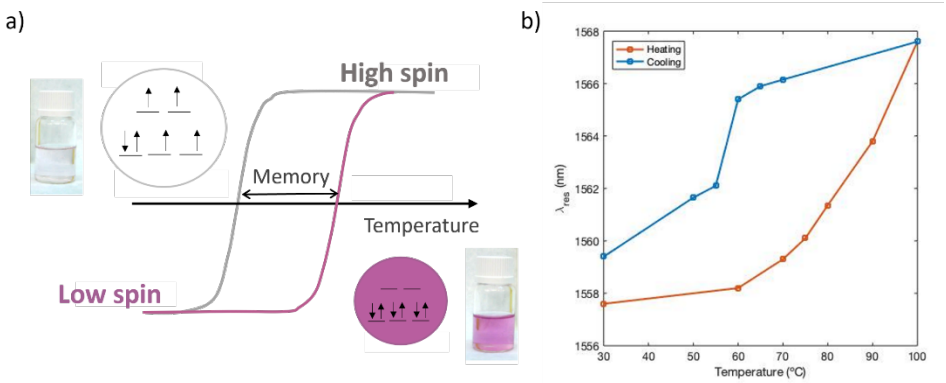

Figure 1: (a) Schematic of the spin configurations and typical spin transition curve with abrupt hysteresis. In the low spin state (LS), electrons are paired, the color of the complex is purple/pink, and the volume is smaller. In the high spin state (HS), the electrons are unpaired, the complex gets a transparent color and the volume increases. (b) Measurement of the optical signal (λr_{es}, resonance frequency) as a function of the temperature where the expected hysterical response is clearly observed.

Periodically driven chiral engine beyond the Carnot limit

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Classically, the power generated by an ideal thermal machine cannot be larger than the Carnot limit. This profound result is rooted in the second law of thermodynamics. Whether this bound is still valid for microengines operating far from equilibrium is an open question in quantum thermodynamics. Here, we demonstrate [1] that a quantum chiral conductor driven by AC voltage can indeed work with efficiencies much larger than the Carnot bound. Our pump engine [see Fig. 1(a)] consists of a scatterer of arbitrary energy-dependent transmission tunnel coupled to electronic hot and cold reservoirs in the presence of an external AC bias voltage. An AC driving typically generates a finite input power that diminishes the efficiency. Our key idea to overcome this difficulty is to selectively apply an AC external field to the electrons depending on the direction, which can be implemented using a chiral conductor such as those created in two-dimensional systems (topological or quantum Hall conductors) [see Fig. 1(b)]. This completely avoids any AC input power, allowing a high efficiency of the quantum engine, in contrast to nonchiral cases. Nonetheless, entropy production is always positive when using the proper definition for AC driven conductors beyond weak coupling [2] and the second law is preserved. The role of the AC driving can be interpreted as a nonequilibrium demon [3] as the driving induces additional entropy production by rearranging the electron energy distribution in a more uncertain way, while injecting zero net energy. Our results are relevant in view of recent developments that use small conductors to test the fundamental limits of thermodynamic engines.

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Figures

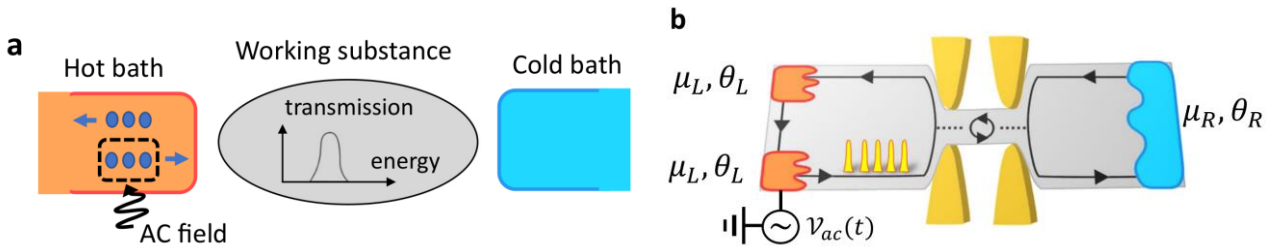

Figure 1: (a) Schematic of periodically driven chiral engine. (b) An implementation using a chiral conductor. $\mu_{L(R)}$ and $\theta_{L(R)}$ are chemical potential and temperature of left (right) reservoir.

Focusing of In-plane Hyperbolic Polaritons in Van der Waals Crystals

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Polaritons -hybrid light-matter excitations- play a crucial role in fundamental and applied sciences, as they enable control of light on the nanoscale [1]. The recent emergence of low-loss van der Waals (vdW) materials opens the door to achieving anisotropic optical phenomena owing to their layered crystal structure, which leads to an intrinsic and strong out-of-plane (perpendicular to the layers) optical anisotropy. A prominent example is given by hyperbolic phonon polaritons (PhPs) -infrared light coupled to lattice vibrations in layered polar materials- in hexagonal boron nitride (h-BN) [2], which exhibit long lifetimes, ultra-slow propagation and hyper-lensing effects. Only recently, PhPs with in-plane hyperbolic dispersion, a key requirement for on-chip planar optical circuitry, have been demonstrated in natural slabs of α-phase molybdenum trioxide (α-MoO3) [3-5] and vanadium pentaoxide (α-V2O5) [6].

In this work, we demonstrate focusing of infrared ray-like hyperbolic PhPs into deep subwavelength focal spots along the surface of α-MoO3 crystals by using metal antennas with an optimized design. Specifically, field confinement is achieved in focal spots with a size of λp/4.5=λ0/50 (λp is the polariton wavelength and λ0 is the photon wavelength in free space). Moreover, the achievable focal distance in in-plane hyperbolic α-MoO3 can be tuned to values well below the diffraction limit in in-plane isotropic materials, along with a better performance in terms of near field confinement and optical absorption. Our findings set the grounds for planar polaritonic technologies at the nanoscale [7].

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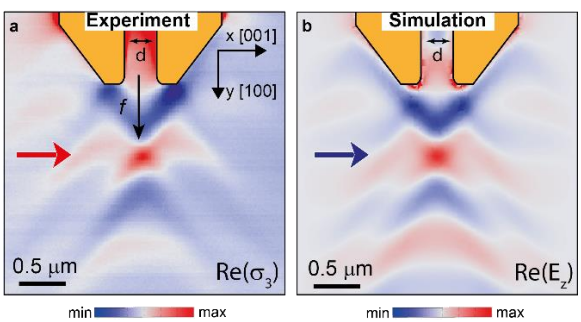

Fig. 1 Nanofocusing of PhPs along the surface of a α-MoO_3 flake into deep-subwavelength focal spots.

Layered hybrid metal-halide perovskites under strain: insights from photoluminescence and micro-Raman spectroscopy

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Layered hybrid organic-inorganic metal halide perovskites (HOIPs) have emerged as promising materials for optoelectronic device applications, namely due to their tunable bandgap and high carrier mobility. For the successful integration of these materials into devices it is key to understand the relationship between composition, crystal structure and optical properties and how to control them.[1] In particular, research has been directed toward the modulation of their optical properties, with special attention on their photoluminescence (PL). Therefore, several strategies have been proposed such as the variation of their organic-inorganic composition[1], or the application of strain[2,3]. Indeed, strain engineering has demonstrated to be an effective strategy to modulate the optoelectronic properties of 2D materials.[4] However, it has been barely explored on HOIPs. Here, we report the tuning of the micro-photoluminescence emission of 2D lead-bromide HOIP flakes subject to biaxial strain. To generate the mechanical strain, we placed the flakes by viscoelastic stamping on a rigid SiO_2 ring platform, leading to the formation of domes (Figure 1a). At low temperatures, we found that a strain < 1% can change the PL emission spectrum from a single peak (unstrained) to three well-resolved peaks (Figure 1b). Combining temperature-dependent micro-PL and Raman spectroscopy mapping (Figure 1c) and reverse mechanical engineering strain modeling, we confirm that the emergence of the two new PL peaks is related to tensile and compressive thermo-mechanically generated strain coexisting along the flake surface and thickness.[5] Our findings provide new insight into strain-based optoelectronic and sensing devices using 2D HOIPs, leveraging on the design of material composition and substrate platform design.

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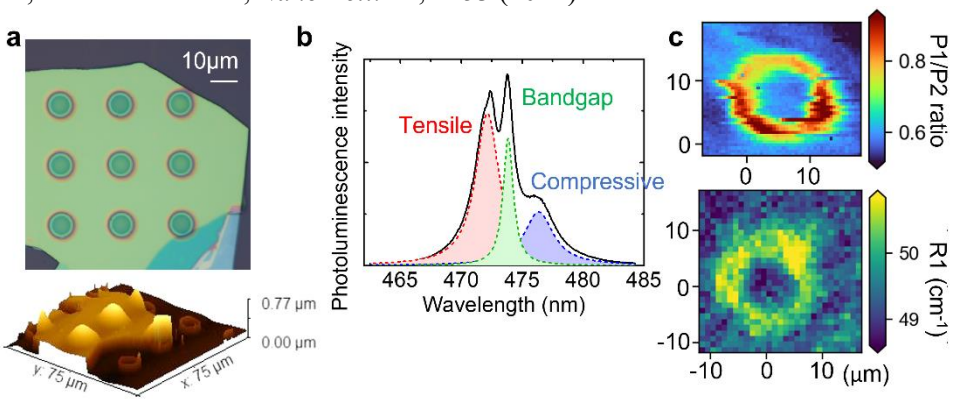

Figure 1: a, Optical microscope image of the flake placed on the rings accompanied by a topography reconstruction of two domes. **b**, Representative photoluminescence emission in the regions close to the ring. **c**, low-temperature photoluminescence and Raman mapping of a dome.

Fundamentals and applications of the voltage-triggered insulator to metal transition

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Many correlated oxides feature an insulator to metal transition (IMT) with a large change of resistivity. Generally, these transitions can also be induced electrically, a phenomenon known as voltage-triggered IMT [1,2]. The associated volatile resistive switching has attracted a lot of attention due to potential applications in optoelectronics, neuromorphic computing or rf switches [3]. Despite the wide interest, the fundamental aspects of this voltage-triggered IMT are not well understood. In this talk I will discuss the underlying physics of this phenomenon [1], including topics such as what governs the characteristic length- and time-scales [2,4].
I will also review the current efforts towards applications, with an emphasis on neuromorphic [3,5,6] and probabilistic computing [7].

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New electrocaloric oxides for sustainable and efficient refrigeration

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As refrigeration is essential for health and comfort, food, medicine or electronics, it represents a large and growing fraction of the worldwide electricity consumption. The current cooling technology, based on the compression of harmful gases, has a limited energy efficiency and contributes significantly to global warming. Caloric effects are among the most promising climate-friendly alternatives because they lead to higher energy efficiencies and use solid refrigerants that can be prepared without toxic elements. Electrocaloric (EC) materials show reversible thermal changes when subjected to variations of an applied electric (E) field, known as the electrocaloric effect (ECE), which maximizes near a ferroelectric phase transition [1]. While the research in their magnetocaloric (MC) counterparts is rather mature, EC materials have been in the spotlight only in the last ten years [2], being advantageous over MC because of the ease of application of E fields. Up to now, the research in EC materials has been dominated by lead-based oxides. Sufficiently large ECE values for cooling applications have only been observed in thin-film samples.
We have investigated new EC oxides (bulk and thin film) by making use of in-house laboratory methods for the "direct" and "indirect" measurements of the ECE, combined with complementary synchrotron-based X-ray absorption spectroscopy. In particular, layer-structured ferroelectric Aurivillius oxides $Sr_{n-3}Bi_4Ti_nO_{3n+3}$ (n = 4, 5), where the A- and B-site of the "n" perovskite-like layers are occupied by Sr/Bi and Ti, respectively. The Curie temperature T_C of their ferroelectric transitions is about 800 K and 560 K for n = 4 and 5, respectively. Aiming at enhancing their EC response at near room temperature (RT), chemical substitutions at the A- (La^{3+}) and B-site (Nb^{5+}) have been applied to tune T_C close to RT. For both series of compounds (n = 4, 5), we found that La-doping is effective in decreasing T_C and in promoting a relaxor ferroelectric behavior but at the expense of weakening the ferroelectricity and EC properties. Preliminary results (Fig. 1) for $Sr_2Bi_4Ti_5O_{18}$ (n=5) show a promising direction towards enhancement of the EC properties through a combination of La- and Nb-doping featuring an ECE maximum close to RT [3].

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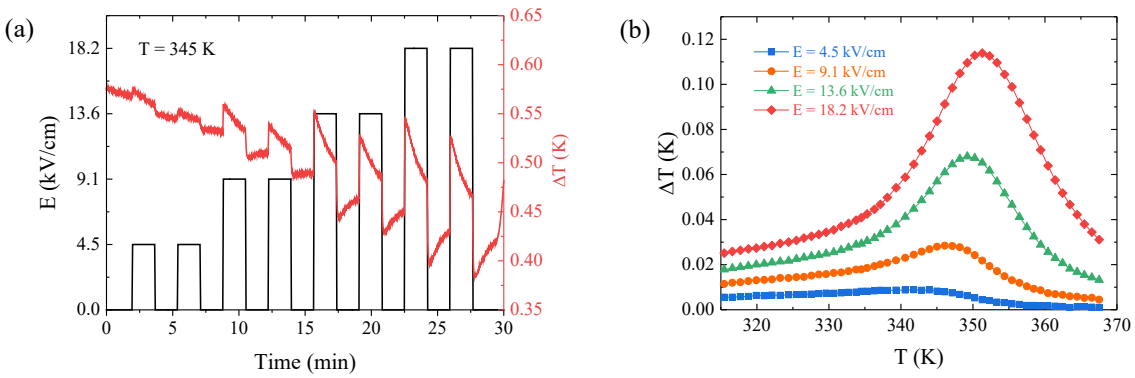

Figure 1. Direct measurements of the ECE temperature change (ΔT), obtained with a quasi-adiabatic calorimeter, for $Sr_2Bi_{3.44}La_{0.5}Ti_{4.8}Nb_{0.2}O_{18}$ at several applied field values. (a) Example of a measurement at T = 345 K as a function of time, and (b) ΔT values as a function of temperature, measured upon heating.

Combining Freestanding Ferroelectric Perovskite Oxides with Two-Dimensional Semiconductors for High Performance Transistors

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Field Effect Transistors (FETs) based on silicon technology are facing limits during the last years. To overcome this obstacle an approach to miniaturize even more the devices can be developed, besides the performance can be improved to lower the power consumption, and thus the heat dissipation. But another approach can be used, which consists of adding new degrees of freedom, such as the polarization in a ferroelectric material, hence the device functionality is increased.

The remarkable properties of 2D materials together with their reduced vertical dimensions, directly positioned them as potential components in FET fabrication [1]. The extensive work, particularly on transition metal dichalcogenides-based FETs have proven their suitability, even surpassing the typical characteristics of the silicon-based transistors [2]. Moreover, the recent development of strategies to isolate complex oxide layers and manipulate them similarly to their van der Waals counterparts has placed new tokens on the board [3,4].

In this work [5], we integrate freestanding single-crystalline $BaTiO_3$ with monolayer MoS_2 flakes, showing mobilities larger than the ones obtained with standard SiO_2 and in the same order of magnitude of devices built with hexagonal boron nitride, which has already shown outstanding electrical properties in FETs [6]. Besides, the devices made with $BaTiO_3$ show a wide hysteresis related to ferroelectric polarization switching in their electrical transfer curves, an appealing property in memory storage devices.

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Extremely long-range, high-temperature Josephson coupling across a half-metallic ferromagnet

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The Josephson effect results from the coupling of two superconductors across a non-superconducting spacer to yield a quantum coherent state. In ferromagnets, singlet (opposite-spin) Cooper pairs decay over very short distances, and thus Josephson coupling requires a nanometric spacer. In systems with particular properties, however, equal spin triplet Cooper pairs can be generated, allowing the coupling of superconductors across magnetic barriers over much longer distances. Despite many experimental hints of triplet superconductivity at ferromagnet/superconductor interfaces, long range triplet Josephson effects across ferromagnetic barriers have remained elusive. We demonstrate extremely long range high-temperature Josephson coupling across the half-metallic manganite $La_{0.7}Sr_{0.3}MnO_3$ combined with the superconducting cuprate $YBa_2Cu_3O_7$. This is shown in planar junctions which display the hallmarks of Josephson physics: critical current oscillations (Fraunhofer pattern) and quantum phase locking under microwave excitation (Shapiro steps). Interestingly, both in the Fraunhofer pattern and in the Shapiro steps, a strong second harmonic can be observed, which further confirms the exotic superconducting state that can be present in this system. [1-3] The marriage of high-temperature quantum coherent transport and full spin polarization brings unique opportunities for the practical realization of superconducting spintronics, and enables novel strategies for devices in quantum technologies.

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Probing and tuning the electronic properties of low dimensional van der Waals materials

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Probing and tuning the electronic transport properties of low dimensional van der Waals (vdW) materials may represent one of the routes that can satisfy the requirements of modern electronics advancements. The low dimensionality of such materials is not only of interest for scalability purposes in electronic applications, but it brings into the game new and exotic physical phenomena, which can also be tailored creating artificial systems with on demand properties, the so-called vdW heterostructures. Following these two ideas, in one part of my thesis, I studied the interplay between the chirality of the Te nanowires, its band structure, and the charge-to-spin interconversion phenomena occurring when electrical current is applied to this low symmetrical structure [1]. The other part of the work, which is presented here, focused on the molecular tuning of vdW materials' properties. We employed hybrid organic/inorganic heterostructures with the idea of exploiting the chemical flexibility of molecular compounds, to obtain functions by design.
In particular, in the first work (Fig. 1 a)) we tailored the superconductivity of single layer $NbSe_2$ via self-assembled molecular adlayers. A programmable modulation of the superconducting critical temperature (T_C) was achieved through carrier density variations induced by strong dipolar interaction developing between $NbSe_2$ and the self-assembled molecular layer [2].
In the second work (Fig. 1 b)), we demonstrate the emergence of a spinterface effect at the interface between prototypical layered magnetic metal Fe_3GeTe_2 and thin films of Co-phthalocyanine. Magnetotransport measurements show that the unpaired spins in Co-phthalocyanine develop antiferromagnetic ordering that pin the magnetization reversal of Fe_3GeTe_2 [3]. In both works the modulation of T_C and the exchange bias induced by the molecules is competitive with the results reported by previous studies trying other approaches, demonstrating the potential of molecular functionalization to tailor the properties of vdW materials.

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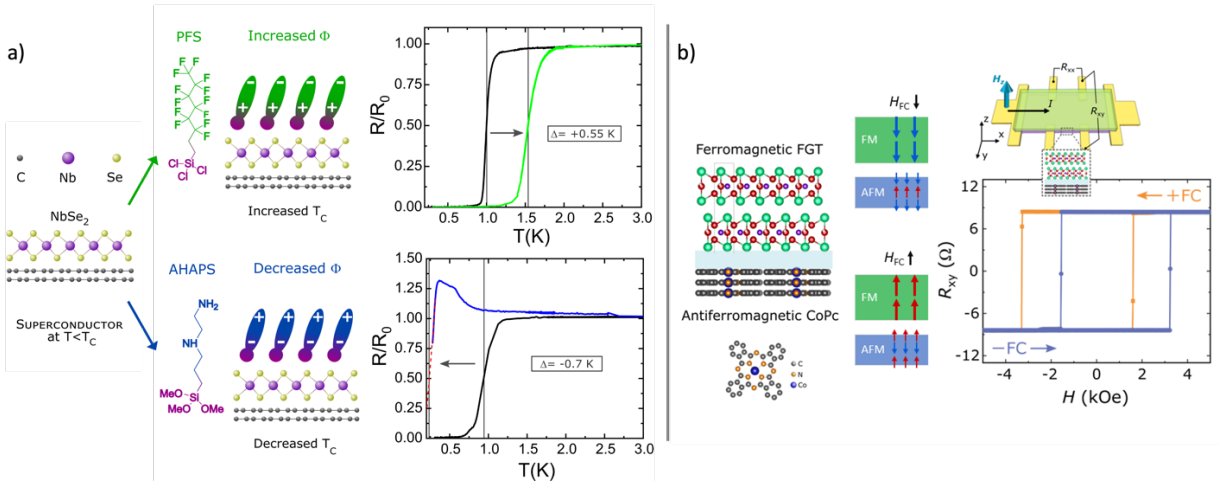

Figure 1: a) Superconductivity modulation in large-area single-layer $NbSe_2$ via self-assembled molecular adlayers. b) Exchange bias in CoPc/Fe_3GeTe_2 van der Waals heterostructure induced by a spinterface effects.

Topological Materials from a Symmetry Perspective

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In this talk I will be presenting the main results of my thesis, mainly the 3 most relevant papers. First, our work on PbTe, a rock-salt structure material that can present a topological transition as a function of hydrostatic pressure. Second, the ferromagnetic pyrite CoS2, a well-studied material that we analyze from the topological perspective, finding nodal lines and Weyl nodes with their respective surface states. Lastly, we explore the role of symmetry in time-dependent elastic deformations of a topological semimetal, which gives rise to a new, purely 3-dimensional hydrodynamic response known as hall viscosity.

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Figures

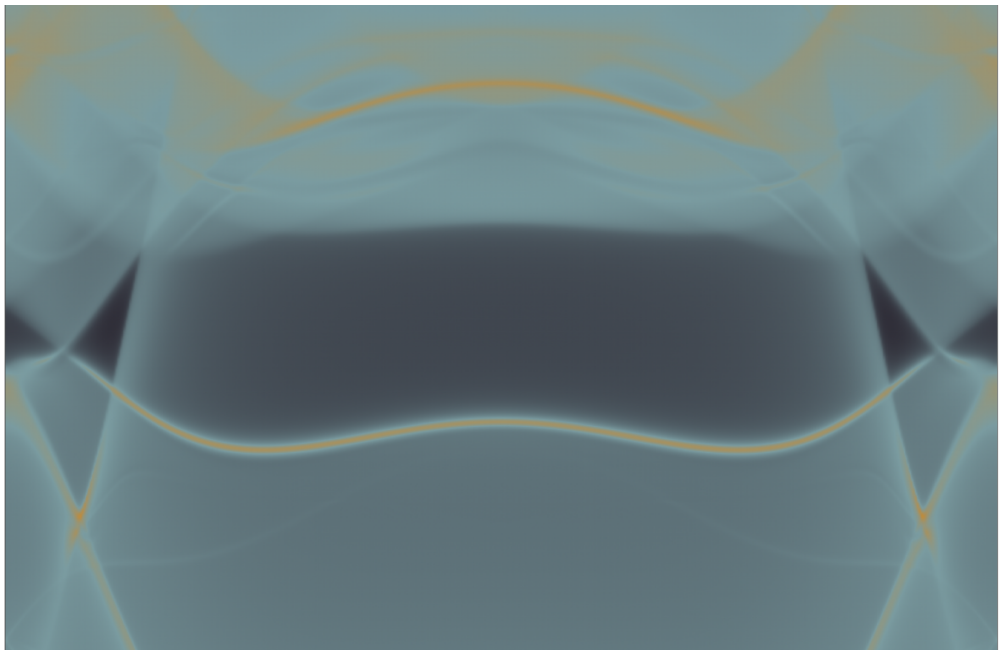

Figure 1: Fermi arcs connecting the projection of Weyl nodes in the (100) surface.

On symmetry and topological aspects of novel phases of matter

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This thesis addresses three classes of topological phases of matter: topological insulators, nodal semimetals and $\mathbb{Z}_2$ topologically ordered states. Their distinctive properties are analyzed combining condensed matter and high energy techniques that depart from their low-energy quasiparticles and their symmetries.

A salient feature of topological insulators is the existence of quantized observables in terms of fundamental constants. By means of effective field theory and tight-binding modeling, we demonstrate that the quantization of circular dichroism in chiral higher-order topological insulators is possible by choosing suitable frequency windows for light absorption.

Nodal semimetals also manifest quantization through the circular photogalvanic effect. We characterize this optical response for the material CoSi by means of a $\mathbf{k}\cdot\mathbf{p}$ analysis to scrutinize its recent experimental observation. These systems are generally described at low energies by small Bloch Hamiltonians; we additionally develop a group theory method to determine any physical observable associated with these finite Hamiltonians without the explicit use of its eigenstates, which allows to avoid unnecessary complications coming from their phase arbitrariness. Finally, we apply renormalization group theory in Weyl semimetals to analyze the emergence of symmetries at low energies under the influence of Coulomb interactions.

In general, intrinsic topological order comes hand in hand with strong correlations that challenge its microscopic study. By exploiting local and global symmetries, we construct ideal models that analytically capture the universal properties of systems with a finite density of $\mathbb{Z}_2$ anyons, conforming whether a Fermi liquid or a Bose-Einstein condensate.

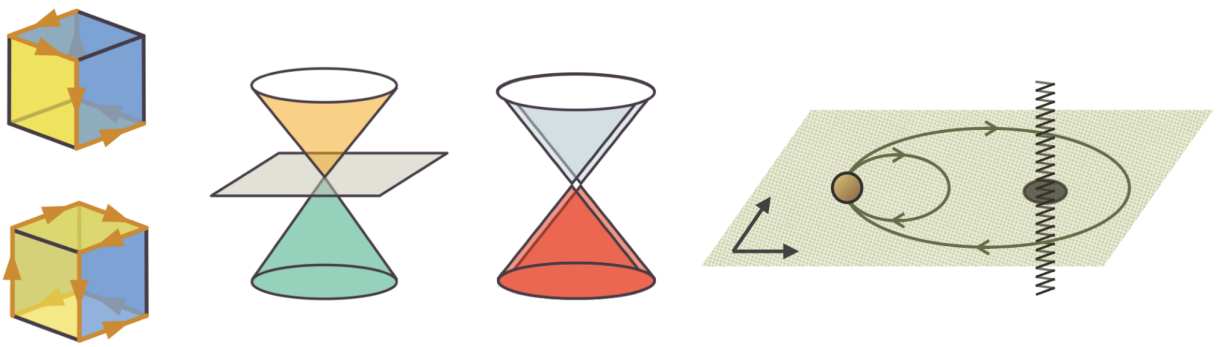

Figure 1: Illustration of the topological phases of matter considered in this thesis.

Quantum devices for thermodynamics at the nanoscale

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As we miniaturize devices to reach the quantum regime, the needs arises to test the laws of thermodynamics in a new realm, in which fluctuations and quantum effects play a very important role. I will discuss how to explore the thermodynamics of the semiconductor devices at nanometer scales, and I will show how we measure the thermodynamic cost of recording the passage of time. We find that the accuracy of our clock and the entropy produced by it are proportional, as predicted both for classical and quantum regimes.

Coupling charge or spin states to mechanical motion might allow us not only to build nanoscale motors but to measure the thermodynamic cost of quantum information processing. Fully suspended carbon nanotube devices allow us to control mechanical, electronic and spin degrees of freedom with high accuracy. Using these devices we find that the coupling of electron transport to the nanotube displacement is ultra-strong. I will discuss how this experimental platform can allow for the study of non-chip quantum energetics.

Visualizing waves and quantum well states at the surface of the heavy Fermion URu_2Si_2.

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Electrons can form a two-dimensional electron gas at metal surfaces, where lateral confinement leads to quantum-well states. Such states have been observed for highly itinerant electrons but remain challenging to visualize in strongly correlated systems because correlations often reduce the separation between energy levels. Here we use millikelvin scanning tunneling spectroscopy to study atomically flat terraces on U-terminated surfaces of the heavy-fermion superconductor URu_2Si_2 which exhibits a mysterious hidden-order state below 17.5 K. We observe two-dimensional heavy fermions (2DHF) made of 5f electrons with an effective mass 17 times the free electron mass. The 2DHF form quantized states separated by a fraction of a meV. Edge states on steps between terraces appear along one of the two in-plane directions, suggesting electronic symmetry breaking at the surface. Our results propose a new route to realize quantum-well states in strongly correlated quantum materials and to explore how these connect to the electronic environment [1].

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Diversity of radial spin textures in chiral materials

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We introduce a classification of the radial spin textures in momentum space that emerge at high-symmetry points in crystals characterized by non-polar chiral point groups (D_2, D_3, D_4, D_6, T, O). These spin textures are an important ingredient to explain the current induced magnetization parallel to direction of the electric field, an effect that might find application in spintronics devices. Based on the symmetry constraints imposed by these point groups in a vector field, we study the general expression for the radial spin textures up to third order in momentum. Furthermore, we determine the high-symmetry points of the 45 non-polar chiral space groups supporting a radial spin texture. These two principles are used to screen materials databases for examples of systems that go beyond the basic hedgehog radial spin texture. As a result, we found that complex radial spin textures given by quadratic and cubic momentum terms are common in the band structure of any material with high-symmetry points having a non-poloar chiral point group. More generally, the symmetry analysis proposed in this work is also valid for studying other vector properties in momentum space.

Extending the spin excitation lifetime of a magnetic molecule on a proximitized superconductor

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Magnetic molecules adsorbed on surfaces serve as a platform to individually address and manipulate spins. In order to be able to use these spins in quantum information processing and data storage, long spin-relaxation times is a prerequisite. Normally, coupling of the spin with the conduction electrons of metallic substrates quenches the excited state lifetime and leads to short relaxation times T_1. However, the presence of superconducting paring effects in the metal substrate can protect the excited spin from relaxation [1]. Upon adsorption on a superconducting surface and depending on the coupling of the unpaired spins with the substrate, several in-gap [2] and outer-gap [3] states may arise, which can be studied with scanning tunneling microscopy and spectroscopy. In this study, we use a substrate of a few monolayers of gold epitaxially grown on top of an oxygen reconstructed 1x5-V(100) surface to decouple the molecular spin of an iron-porphyrin-chloride from itinerant electrons. The gold film exhibits a proximitized superconducting gap with in-gap de Gennes-Saint James resonances, which protects molecular spin excited states and results into a lifetime of $\tau \approx 80$ns. The spin lifetime decreases with increasing film thickness due to the gradual gap-closing by the in-gap states. Our results elucidate the use of proximitized gold electrodes for addressing quantum spins on surfaces, envisioning new routes for tuning the value of their spin lifetime.

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Figures

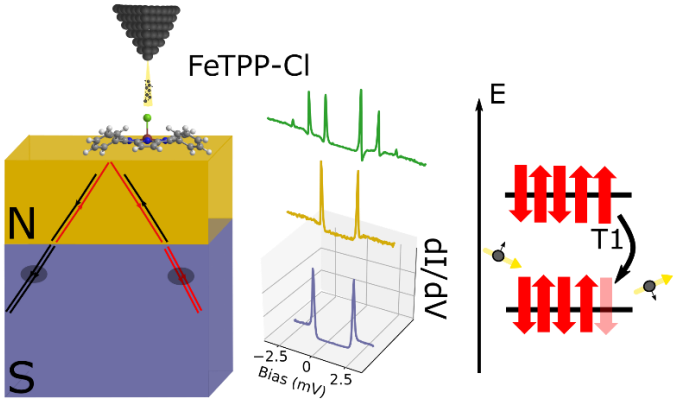

Figure 1: Left: Artistic description of the molecule/normal metal/superconductor system, **Center**: Corresponding spectroscopic signatures, **Right**: Illustration of a spin-flip excitation on the magnetic center induced by tunneling electrons

Real-Time Second Principles TD-DFT calculations of Optical Properties: Can large-scale methods be used to simulate Excitons?

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Research on solid-state spectroscopy is essential in the development of novel technological applications based on energy and charge transport. The phenomena observed in spectroscopy cover many topics in condensed matter as it is affected by the presence of impurities, distortion of the lattice (phonons) or electron scattering, and the results can be strongly dependent on the boundary conditions like strain or temperature. Analyzing the information obtained from experimental spectra can be difficult and supporting from *ab initio* calculations can be quite useful to interpret and understand the observations. However, this task is also a challenge as these simulations would require in many cases, large supercells, detailed sampling of atomic movement/impurity localization or require the use of advanced computational techniques to account for electron-electron and electron-hole correlations.

Therefore, it would be desirable to go beyond the capabilities of standard first principles methods to carry out predictive large-scale simulations. This fact motivates the development of a new family of methods, known as Second Principles (SP) [1], based on Density Functional Theory (DFT) and implemented in the code SCALE-UP. They allow large-scale material-simulations, including both atomic and electronic degrees of freedom, at a very modest computational cost. The method is based on the construction of models written in localized Wannier functions [2] and includes the capacity to describe the changes in the electronic state induced by the application of electric fields, variations in the geometry (including electron-phonon coupling) and the electron density itself (electron-electron scattering).

In this work, we show the results obtained by combining (i) the newly developed code to generate SP models, named MODELMAKER, and (ii) our implementation of real-time time-dependent DFT. Using our model generator, and based on hybrid DFT simulations, we are able to create models that take into account strong electron-electron interactions. Combined with our efficient algorithm to evolve the density matrix in real time (RT), we discuss the influence of these interactions after the system has been perturbed by a short electric pulse. Initial results show that electron-hole interactions have a strong influence on the resulting spectrum, and can be seen using our novel computational technique, unlike what happens in standard linear response TD-DFT calculations. This fact, indicates that RT-TD SP simulations could be a new powerful tool to study excitons at a computational cost much smaller than the one of the current methods like the Bethe-Salpeter equation.

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Synchrotron X-ray Coherence to Probe the Complexity of realistic interfaces at the Nanoscale

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The advent of the world's first coherent hard X-ray sources in France (ESRF) and the USA (APS) represents an unprecedented opportunity to conduct operando (i.e., in situ and time-dependent) studies on the structure and behavior of surfaces, interfaces, and single crystalline grains in reactive environments. In this talk, I will give an overview of the new approaches utilizing x-ray coherent scattering to observe the structure of crystalline matter in three dimensions and with special sensitivity to nanoscopic defects, lattice distortions, irregular morphologies and their evolution under experimental conditions mimicking natural environments. As an example, I will describe our recent studies about growth and dissolution at mineral-water interfaces with coherent x-rays. In the first study coherent X-ray reflectivity was used to reveal the morphology and the active sites for growth and dissolution of a an otavite ($CdCO_3$) thin film grown on a dolomite substrate [1]. The second study shows a novel approach to extract structural information from a coherent diffraction pattern based on the re-interpretation of the Patterson Function as an auto-hologram and a mathematical graph [2]. These two studies form the initial basis of a research program aiming to develop advanced coherent x-ray imaging methodologies to characterize the dynamic and chemical behavior of crystalline grains at the nanoscale and under realistic environments (e.g. mineral matrices, multilayered compounds, liquid solutions, etc.).

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Quantifying the magnetic anisotropy of 50 nm-magnetic nanoparticles embedded in biological entities

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Over the last years, the interest in nanomagnets have blown up aiming to overcome the fundamental need to develop novel nanotechnology-based pathways to achieve relevant performance in medicine. On the top of their reduced size, (comparable to those of proteins, nucleic acids, or viruses) that allows promising interaction with biological systems, the magnetic nature of the nanomagnets grants their manipulation by external magnetic fields. All of it makes magnetic nanostructures excellent candidates to be used as diagnostic agents, to locally heat and destroy cancer cells in hyperthermia cancer treatment or for targeted magnetic cell delivery in regenerative medicine [1]. All these applications rely on the underlying physical properties of the nanomagnets within the target biological entity. In particular, the role of the magnetic anisotropy arises an overriding question [2]. Despite its importance, the quantification of the magnetic anisotropy of in individual magnetic nanostructures is a challenging task. Commonly used macroscopic magnetic characterization techniques average over hundreds or thousands of dissimilar nanomagnets, impeding to obtain reliable information about magnetic anisotropy of individual nanostructures. Regardless of the existence of magnetic sensitive microscopic methods, they are either limited in spatial resolution or in magnetic field strength or more relevant, they do not allow to measure magnetic signals of nanomagnets embedded in biological systems.

Here we present a hybrid experimental/theoretical method capable of working out the magnetic anisotropy constant and the magnetic easy axis direction of individual magnetic nanostructures down to 50 nm embedded in biological entities [3]. The method combines experimental data acquisition by means of scanning transmission x-ray microscopy using an axi-asymmetric magnetic field with theoretical simulations based on the Stoner-Wohlfarth model. The validity of the method has been tested over a model system consisting of single-domain intracellular magnetite nanoparticles biosynthesized by magnetotactic bacterium *Magnetovibrio blakemorei* MV-1. Magnetotactic bacterium MV-1 synthesize internally high-quality truncated hexa-octahedral magnetite (Fe_3O_4) nanoparticles with dimensions 35x35x65 mm arranged in chains. The elongated morphology of such particles along the chain direction (<111> direction), yields a strong effective uniaxial magnetic anisotropy along that direction [4]. As a consequence, the nanoparticles biosynthesized by *M. blakemorei* are uniaxial single magnetic domains whose magnetization process can be described by a modified Stoner-Wohlfarth model.

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Nanogenerators and self-powered sensors enabled by plasma and vacuum processing of multifunctional thin films and 3D nanoarchitectures

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Single- and multi-source environmental energy harvesters and nanogenerators will promptly pave the way for the realization of Industry 4.0 and Smart Cities. However, advances are yet required in the design of functional nanomaterials, and their synthesis and processing procedures. In this presentation, we will demonstrate the application of vacuum and plasma-assisted deposition techniques to process surfaces and thin films and to develop complex nanowires (NWs) and nanotubes (NTs) with a core@multishell morphology where each shell adds functionality or multifunctionality to the system. The steps required for the implementation of these nanomaterials as supported or in-device applications will be presented together with our latest accomplishments in the field of solar cells,[1-4] piezoelectric and triboelectric nanogenerators[5,6] and self-powered sensors.

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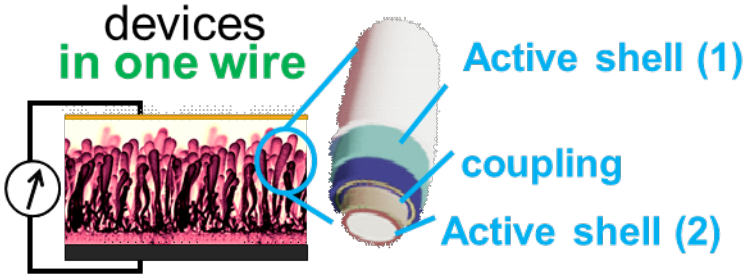

Figure 1: Schematic representation of a high-density array of multifunctional nanowires for multi-source energy harvesting.

STM Study and Electronic Transport Signature of Dithiahelicenes at Ambient Conditions

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Using a Scanning Tunneling Microscope (STM), we address the chiral molecules dithia[*n*]helicenes ([*n*]DTH, being *n* = 7, 9 and 11 the number of rings) in benzene solution [1, 2]. For each [*n*]DTH, two kinds were synthesized where the location of both sulfur atoms changes. This fact leads to different anchoring preferences.

For this work, Au(111) substrates were selected for studying the self-assembly of helicenes over the surface. First result shows differences during the deposition due to the interaction of the sulfur atom as a link group with the gold atoms. Moreover, we could image isolated molecules along their different binding configurations, measure the molecular diameter and establish a chiral recognition method at room conditions.

By means of STM-based BJ, we performed electronic transport measurements which show the most repeated conductance values when stretching the junction up to the formation of a molecular bridge.

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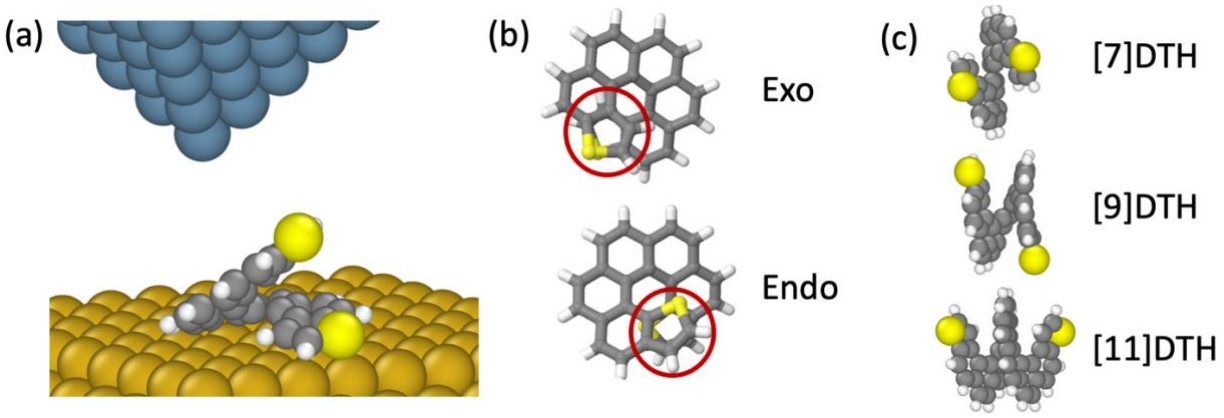

Figure 1: (a) Schematic illustration of an STM set up where a helicene is flat over a Au(111) substrate and the tunneling current is measured via a PtIr tip. For measuring via STM-based BJ, the tip is changed to a gold wire. Molecules are represented with grey, white and yellow spheres as C, H and S atoms respectively. The location of the sulfur atom is highlighted using a red circle for the exo and endo compounds in panel (b). Panel (c) shows a side view of one molecule as a function of *n*, being *n* = 7, 9 and 11 rings.

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Spatial control of the thermal conductivity in transition metal oxides

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Atomic point defects are one of the main sources of phonon scattering, and hence of the limiting factors of thermal conductivity in non-metallic crystals [1,2]. In the case of transition-metal oxides, an unavoidable number of ionized oxygen vacancies are formed during synthesis and remain randomly distributed along the crystal.
In some oxygen-deficient perovskites, previous experiments demonstrated that the electric field produced by a voltage-biased atomic force microscopy tip can induce a transformation between the perovskite and a brownmillerite phase at room temperature, with sub-micrometer spatial resolution.[3]
Here we show that such transformation can be exploited to produce different thermal conductivity states. In particular, we show that the thermal conductivity of several oxides can be modified ≈ 30 % at room temperature, with micron-size spatial resolution. This shows that ionic-based thermal devices can be fabricated by electric-field patterning.

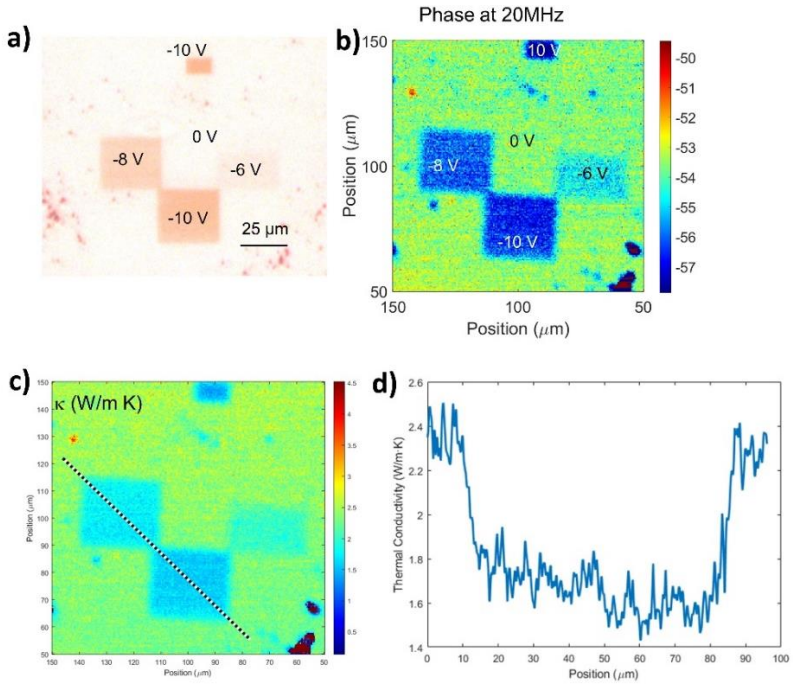

Figure 1: a) Atomic Force Microscopy image of a thin film of $SrFeO_{3-x}$ deposited on STO. The dark squares have been scanned with a voltage-biased AFM tip, dragging oxygen vacancies and inducing the local transformation to the browmillerite $SrFeO_{2.5}$ phase. b) Frequency Domain Thermoreflectance Phase at 20 MHz obtained in the same region as a). In c) we show the thermal conductivity map obtained from the fitting of the reflectivity map. d) thermal conductivity along the dotted line shown in c).

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