# Collection of Abstracts

## OEM-2D Workshop
## San Sebastian 2024

# Keynotes & Invited Speakers

# Eva Andrei: tbd

# Exploring Chiral Spin States in Curved Spaces: Insights from Ring Geometries

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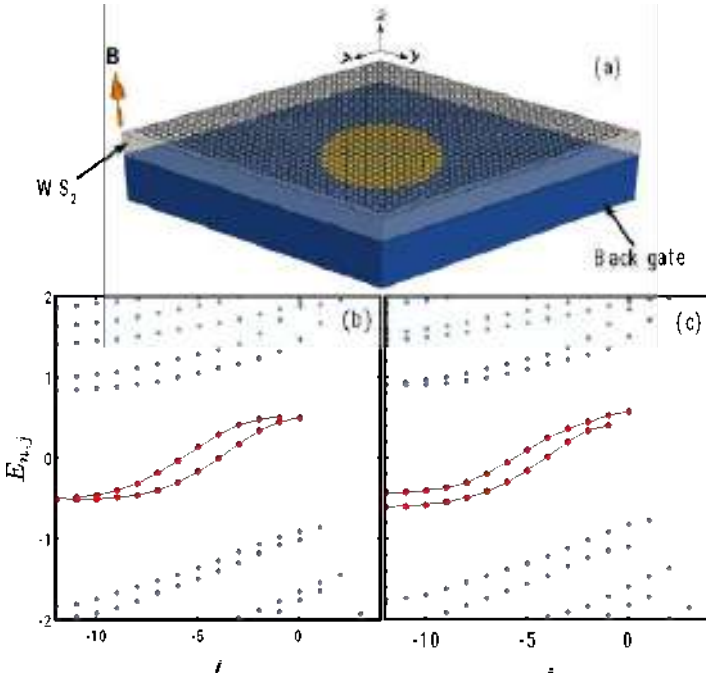
In this presentation, I will review the problem of electron spins moving in curved spaces, focusing on the problem of ring geometry. I will then demonstrate how chiral states in circular graphene *pn* junctions, subjected to normal magnetic fields and strong proximitized spin-orbit coupling, can imitate those of propagating spin carriers in semiconducting quantum rings. I will derive the effective one-dimensional Hamiltonian governing the spin dynamics of the zero modes and calculate the associated geometric phase. I will also show that for a given polarity of the junction, a special point exists in parameter space where the spin is completely polarized along the radial direction in the graphene plane. Additionally, I will propose a novel quantum-Hall interferometer setup that can readily identify and observe these remarkable features. By employing this interferometer, I can gain valuable insights into the intricate nature of chiral spin states and their manifestation in ring geometries.

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# Linear spectroscopy of collective modes and the gap structure in two-dimensional superconductors

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We consider linear optical response in multi-band, multi-layer two-dimensional superconductors. Within a simple model, we show that Leggett and clapping modes can be detected in linear response, and show how trigonal warping of the superconducting gap can ease detection of the clapping modes. Taking rhombohedral trilayer graphene as an example, we consider several tentative pairing mechanisms and show that all-electronic mechanisms may produce additional collective modes relative to the conventional (phonon) mechanism. Lastly, we show that even neglecting collective modes, the linear response contains a wealth of information about the superconducting gap structure. Our results suggest that linear spectroscopy can be a powerful tool for the characterization of unconventional two-dimensional superconductors.

# 2D straintronic adaptable photodetectors and transistors

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Strain engineering is an interesting strategy to tune a material's electronic properties by subjecting its lattice to a mechanical deformation. Conventional straining approaches, used for 3D materials (including epitaxial growth on a substrate with a lattice parameter mismatch, the use of a dielectric capping layer or heavy ions implantation) are typically limited to strains lower than 2% in most cases due to the low maximum strains sustained by brittle bulk semiconducting materials. Bulk silicon, for example, can be strained only up to 1.5% before breaking. Moreover, these straining approaches induce static deformations of the semiconductor materials and therefore they are not suitable for tunable functional devices. 2D materials can be literally stretched, folded, bent or even pierced. [1] This outstanding stretchability (and the possibility of using dynamically varying strain) of 2D materials promises to revolutionize the field of strain engineering and could lead to "straintronic" devices – devices with electronic and optical properties that are engineered through the introduction of mechanical deformations.

In this talk I will discuss our recent efforts to study strain engineering in 2D materials and to exploit it to fabricate strain tunable functional optoelectronic devices. [2-10].

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# Nontrivial topological properties of pentagonal 2D $PdSe_2$

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The theoretical proposal of a pentagonal 2D form of carbon, penta-graphene [1], has stirred the exploration of layered materials composed of pentagons [2]. Among these, palladium diselenide ($PdSe_2$) is gaining increasing attention due to its experimental synthesis and air stability [3]. It has excellent optical and thermoelectric responses; theoretically, pentagonal monolayer and multilayer $PdSe_2$ have been studied extensively by first-principles methods [2,3,4]. We have carried out a detailed analysis of the band connectivity and of the symmetry-related topological properties of this material, relating its electronic and optical properties, which could be measured, to a nontrivial behavior. We report a strong topological phase with a $Z_2 = 1$ phase that appears in the lowest set of conduction bands; this phase is protected by the combined action of time-reversal and crystalline symmetries [4]. In addition, we have found that the electronic structure of its valence bands involves an atomic obstructed insulator related to higher-order topology, which is a consequence of the selenium-selenium bond dimerization, along with inversion and time-reversal symmetry. We have also characterized the electronic corner states associated with the atomic obstruction and compute the corresponding corner charge for a finite geometry, which is found to be not quantized but still inversion-protected. These robust topological signatures can be experimentally verified and tuned by strain [5].
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# Quantum and nonlinear plasmonics with 2D materials

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Plasmons—collective excitations of the free electron plasma—constitute nanoscale optical resonators that are imbued with a nonlinear response by their supporting conductive media. In the 2D limit represented by atomically thin materials, plasmon resonances provide unprecedented levels of optical field confinement, while exhibiting relatively lower losses in pristine samples. The appealing properties of 2D plasmons are ideal for nonlinear plasmonics, which seeks to overcome the weak nonlinear response of available materials by exploiting the large near field enhancement supplied by plasmon resonances. Here we theoretically explore nonlinear light-matter interactions of 2D plasmons hosted in atomically thin materials and their heterostructures. Our investigations are based on nonclassical methods to describe graphene plasmons characterized by high confinement and electrical tunablity [1], plasmons supported by ultrathin crystalline noble metal films with thickness-dependent properties and lower losses than their amorphous counterparts [2], and nanostructured phosphorene [3], an anisotropic 2D semiconductor that hosts plasmons in highly-doped samples. We further explore possibilities to trigger nonlinear light-matter interactions on the few-plasmon level [4], and to enhance harmonic generation through synergetic interactions between plasmons in actively tunable graphene heterostructures [5].

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# Exciton polarization in 2D TMDs

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In this talk, I will report two related experiments on the polarization of excitons in monolayer TMDs. With photocurrent experiments, we demonstrate that the in-plane electric field leads to a significant orbital hybridization of Rydberg excitonic states with different angular momentum, especially orbital hybridization of 2s and 2p and consequently optically actives 2p-state excitons. In another excitation intensity dependent photoluminescence experiment, We elaborate the exciton Coulomb screening effect arising from exciton-exciton interaction. We attribute this exciton-exciton interaction to the mutual polarization instead of the conventional Coulomb exchange interaction.

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# Proximity effects in van der Waals materials

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Graphene has weak spin-orbit coupling and no magnetic order. But when placed in contact with a strong spin-orbit coupling material, such as a TMDC, or a ferromagnet, such as Cr2Ge2Te6, Dirac electrons acquire strong spin-orbit or exchange coupling, respectively. Such proximity effects render graphene suitable for spintronic applications that require spin manipulation [1]. Graphene with strong proximity spin interactions can host novel topological states [2], or form ex-so-tronic devices [3] which offer spin swap functionalities: switching spin-orbit and exchange coupling on demand by gate. I will review the recent developments in the proximity phenomena in graphene, and present new theoretical results on the control of the proximity spin-orbit and exchange coupling by twisting the van der Waals layers [4, 5]. Finally, I will also discuss the emergence of new correlated phases in graphene [6] due to the presence of proximity spin-orbit and exchange couplings, and the routes towards radial Rashba interactions [7].

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# Andrea Ferrari: tbd

# Nonlinear optical probing and control of magnetic order and electronic band topology

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Illuminating a material with light can reveal both interesting aspects of electronic and lattice degrees of freedom, as well as drive phase and topological transitions in the material itself. In this talk, I will focus on three distinct responses of a material to light: (1) Nonlinear phononic control of magnetism in bilayer $CrI_3$, $MnBi_2Te_4$, and $MnSb_2Te_4$. (2) The non-linear photogalvanic response of Weyl semimetals with tilted cones and chiral charge up to 4 (the largest allowed in a lattice model), as well as the topological superconductor candidate 4Hb-$TaS_2$, and (3) The coupling of phonons to electronic degrees of freedom to produce chiral phonons with large g-factors of order 1, which can be measured with Raman scattering. For nonlinear phononic control of magnetism, I will show how intense THz light can be used to transiently modify magnetic exchange constants, including their sign. In the case of the non-linear current response of Weyl systems, I will review how the quantum geometry—and quantum metric in particular—produces a quantized response proportional to the chiral charge of the Weyl node. I will compare the predictions of low-energy theories with the full band structure for few and multi-band systems, and present new analytical results for chiral charge 4. For the case of a superconductor, I will show how the second order optical response can be used to distinguish topological and non-topological phases of matter. In the case of chiral phonons, I will present a theory for the "giant" g-factors in insulating transition metal oxides based on atomic transitions of the transition metal ions. I will review relevant experimental results before turning to the theory.

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# Electron quantum optics with graphene nanoribbons

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The exploration of atomically-precise graphene nanostructures, particularly graphene nanoribbons (GNRs), has dramatically enhanced our capability to engineer exotic electron and spin states at the quantum level [1], thanks to advanced on-surface synthesis techniques [2]. This talk will outline the computational progression from the initial discovery of electron beam splitting in junctions of crossed GNRs [3-5], through to complex multiterminal transport simulations that facilitate spin filtering [6] and the implementation of Mach-Zehnder-like interferometry within GNR networks [7]. These developments pave the way for promising applications in electron quantum optics, while also laying the groundwork for future innovations in spintronics and quantum technologies. This journey highlights the integration of computational science and quantum physics, unveiling new pathways for manipulating electron dynamics in nanostructured devices.

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# Fast Descriptors and Accelerated Process Development for 2D materials

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We systematically explore nucleation, crystal growth and process mechanisms for thin films and 2D materials at the atomic monolayer limit using CVD-based approaches coupled to new process vectors such as catalytic enhancement.[1,2] For much-needed accelerated materials development, there is demand for characterisation approaches that can both resolve complex structure-property relations down to the atomic detail [3] as well as enable smart, high throughput screening.[4,5] This talk will focus on two such approaches based on imaging spectroscopic imaging ellipsometry (SIE) and scanning electron microscopy. We adapt a Kramers-Kronig constrained variational fitting algorithm for SIE to demonstrate non-destructive, efficient characterisation and scalable mapping of multi-layer semiconductor heterostructures with 1 µm lateral resolution. This methodology proves highly accurate for the model system of $HfS_2$ oxidation, enabling ready access to buried $HfS_2$ layers, oxide quality, and lateral and vertical uniformity. We demonstrate operando capability for thermal $HfS_2$ oxidation up to 400◦C, providing insights into the temperature and time dependent nature of self-limiting oxide growth, as well as the trapping and eventual release of sulfur reaction products. We show that planar imaging with conventional SEM can give a very strong secondary electron contrast between prevalent van-der-Waals epitaxial orientational alignments as well as non-epitaxial mono-layer h-BN domains deposited on Ni(111), thereby opening powerful orientational and film texture mapping capabilities. We demonstrate how this can be used to systematically explore mono- and bi-layer h-BN film texture evolution, from isolated domain nucleation to full coverage, including the resulting domain boundary structures. We also demonstrate high-throughput operando SEM to directly interrogate the mechanisms of catalytic 2D formation including salt-assisted $WS_2$ layer CVD. We thereby employ increasingly automated, machine-learning assisted analysis and parameter space exploration.

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# Exciton, charge and spin lattices in moiré heterostructures

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Vertical semiconductor van der Waals heterostructures with near-resonant band alignment and non-commensurate lattices such as MoSe2/MoTe2 [1] and MoSe2/WS2 [2] constitute peculiar model systems for excitons, charges and spins localized on moiré lattices. Being robust against mesoscopic lattice reconstruction [3] due to sizable lattice mismatch, they exhibit canonical periodic moiré potentials, while near-resonant band alignment induces hybridization of exciton states across the constituent layers. Using cryogenic optical spectroscopy of moiré excitons, we study the effects of correlated charge and spin ordering in such moiré heterostracks with different twist-angle configurations, highlighting emergent magnetism phenomena on effective monolayer and bilayer Hubbard triangular lattices [4]. Moreover, by employing open cavities, we establish the regime of strong light-matter coupling of neutral moiré exciton-polaritons and charged moiré polaron-polaritons, and demonstrate how phenomena of correlated magnetism map onto these exotic light-matter states.

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# News from the Quantum Twisting Microscope

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In this talk I will present the latest results from the Quantum Twisting Microscope1 (QTM), a fundamentally new type of scanning probe microscope, capable of performing local quantum interference measurements at a twistable interface between two quantum materials. Its working principle is based on a unique tip, made of an atomically-thin two-dimensional material. This tip allows electrons to coherently tunnel into a sample at many locations at once, with quantum interference between these tunneling events, making it a scanning electronic interferometer. With an extra twist degree of freedom, our microscope becomes a momentum-resolving local probe providing powerful new ways to study energy dispersions and collective modes in quantum materials. I will present some of our latest experiments with a QTM operating at T=4K, revealing intriguingly strong electron-phason coupling in twisted bilayer graphene and mapping the electrostatic landscape in moiré lattices.

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# On the robustness of gapless states in gated multilayer graphene

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Gated multilayer graphene exhibits topological gapless states localized at interfaces between two different stacking orders. The stacking order change can be created when some layers are stretched, corrugated, or delaminated. Most typically the stacking domain walls occur along the zigzag direction. In this case, the energy valleys in the k-space are well separated. The gapless states are therefore valley-protected and provide one-dimensional non-destructive valley currents that can flow along the stacking domain wall. Valley protection can be destroyed in the presence of atomic-scale defects. Here, we demonstrate the robustness of the gapless states to different defect-like perturbations of the multilayers. It is shown that some gapless states survive very strong distortions of the stacking domain walls. They persist when some layers are broken or partially removed, or even when vacancies or magnetic impurities are present at the stacking interface.

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# Optoelectronics of graphene moiré systems

**Frank Koppens**

*ICFO*

# Understanding the Interlayer Coupling in 1T/1H-$NbSe_2$ Hetero-Bilayers

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The electronic and magnetic properties of two-dimensional (2D) materials are significantly influenced by their underlying substrates, resulting in a range of proximity effects including screening, charge transfer, and hybridization. Despite the critical importance of these effects, theoretical investigations remain sparse. Previous studies on the Star of David (SOD) structure in 1T-NbSe2 predominantly examined configurations without realistic substrates, focusing either on single layers or stacking with homogeneous 1T phases.

In this work, we examine how proximity effects modulate the electronic and magnetic properties of the 1T-NbSe2 phase when interfaced with a metallic 1H-NbSe2 substrate. Employing Density Functional Theory (DFT), we establish a framework to delineate the essential properties of both standalone 1T-NbSe2 and its 1H counterpart. Our analysis reveals the optimal stacking configuration between these layers, highlighting a significant charge transfer of 0.17 electrons from the 1T to the 1H phase and subsequent intra-layer charge reorganization.

Our findings suggest that while the magnetic moment of the SOD structure remains robust, it is attenuated due to a reduction in the on-site Coulomb interactions within the Hubbard bands. Furthermore, the interlayer coupling not only induces metallicity in the 1T phase but also promotes a more pronounced decoupling of the lower Hubbard band from the valence band.

This investigation is one more example of the intricate dynamics between 2D materials and their substrates, providing essential insights into the electronic and magnetic behavior of these complex systems.

# Local field effects in ultrafast light–matter interaction revealed by nonlinear spectroscopy of monolayer materials

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I will present experimental and theoretical investigations on the nonlinear optical response of 2D transition metal dichalcogenides, in particular $MoSe_2$. Nonlinear spectroscopy reveals the dynamics of optically excited occupations and coherences in the temporal and spectral domains, allowing one to access the relevant decay times and homogeneous line widths and thus yielding the information beyond this available from linear spectroscopy [1]. In 2D materials, the optical response is affected by mutual interactions between the optically created excitons, which can be accounted for on the mean-field level by a local-field theory [2-4].

In this presentation I will first discuss the local field effects manifested in the pump-probe spectroscopy of hBN-encapsulated $MoSe_2$ [2]. By comparing experimental results to a theory based on two- and three-level effective models with local fields we show that the latter induce a blue shift of the exciton line by a few meV. In addition, by investigating spectral line widths and amplitudes we can study the influence of excitation-induced dephasing. We find that both effects approximately have the same strength and also influence the appearance of spectral oscillations for an inverted pulse ordering. Next, I will outline the theory of the photon echo in the coherent four-wave mixing response accounting for the local field effects [3]. Finally, I will discuss the experimental observation and theoretical modeling of the new effect of *destructive photon echo* in six wave mixing spectroscopy of $MoSe_2$, which is due to the interference between different orders of local-field interactions [4].

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# Collective optical modes in two-dimensional arrays of nanoparticles

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Two-dimensional periodic arrays of metallic nanostructures can support collective optical 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 [1].

In this contribution, we will discuss some recent theoretical advances on the topic of lattice resonances. In particular, we will explain how the interplay between the response of the individual constituents of the array and their collective interaction determines the ultimate limits of the near-field enhancement provided by lattice resonances as well as their quality factor [2]. We will also discuss the response of arrays with multi-particle unit cells using an analytical approach based on hybridization theory [3], which provides a simple and efficient way to design periodic arrays with engineered properties [4,5]. Furthermore, we will explore how the response of a periodic array is affected by the characteristics of the source used to excite it [6-8]. Finally, we will analyze different array geometries that support lattice resonances with extraordinary properties such as perfect circular dichroism [9] and perfect absorption [10].

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# Superconductivity from electronic interactions on a fragmented Fermi surface

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The alternative mechanisms for the superconducting pairing have been explored for a long time – starting from the Kohn-Luttinger proposal in 1965, through the physics of high-Tc superconductors, up to the recent studies of superconducting pairing in the van der Waals material NbSe2 [1,2]. The common feature of many of these works is that the superconducting correlations between the members of a Cooper pair don't have to arise from an effective attraction, but can be the result of two or more competing repulsions.

The Fermi surface in NbSe2 is split into three pockets, around the Gamma, K and K' points. The presence of different pockets divides the Coulomb scattering processes into subsets with different scattering ranges. The competing repulsion events at different ranges can result in the formation of Cooper pairs, provided that the short-range repulsion is stronger than the long-range one. Depending on which of the interaction types is dominant, we find that the material can support several superconducting gaps with different symmetries, both in the s and in the f pairing channel. We analyze the dI/dV characteristics of recently performed STM experiments on NbSe2 [3] and find that while they are consistent with both one and two gaps, the agreement is better when two gaps are considered.

In order to gauge the strength of the interaction at different ranges we have calculated the screened Coulomb potential in this material, using the tight-binding model and the RPA approximation. We find that while the gaps at K/K' points can form in the absence of the Gamma pocket, once it is included it can be a powerful player, even to the point of changing the symmetry of the gaps in the K/K' valleys.

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# Superconductivity and strongly correlated phases in (un-)twisted graphene multilayers

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# Light-matter interaction in van der Waals crystals and molecules

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Phonon polaritons – lattice vibrations coupled to electromagnetic fields – in van der Waals (vdW) materials can enhance light–matter interactions at mid-infrared frequencies, owing to their extreme field confinement and long lifetimes. Particularly, in some crystals, such as h-BN or MoO3, the dispersion of polaritons – the relation between their momentum and energy – can take a hyperbolic shape and lead to the directional propagation and strong field confinement. The latter is beneficial for coupling between polaritonic fields and molecular vibrations in adjacent organic layers. In this talk we demonstrate that vibrational strong coupling can be achieved between phonon polaritons either freely propagating along vdW crystal layers [1] or "locked" inside resonant cavities [2] and molecular excitations. Such interaction can take place simultaneously in different frequency bands, e.g. at visible and mid-infrared frequencies [3]. We will show the most recent experimental and theoretical studies on the interaction between hyperbolic polaritons and molecules, discuss their applications and future perspectives.

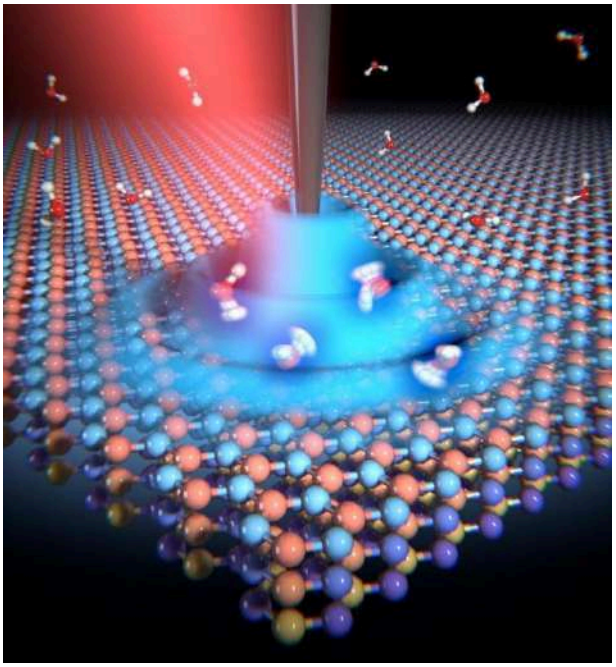

**Figure 1**: An artistic image of a phonon polariton in a vdW crystal layer interacting with molecular vibrational resonances. The vertical rod represents the AFM tip of a near-field optical microscope, probing the interaction.

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# Magnetic properties of orbital Chern insulators in graphene moiré heterostructures

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Moiré superlattices, which arise from small rotational misalignment between layers in van der Waals heterostructures, provide a powerful way to control the interactions and topology of electronic bands. For example, small-angle twisted monolayer-bilayer graphene (tMBG) features narrow moiré minibands with Chern numbers that could be tuned by the electric displacement field. My talk will focus on quantum anomalous Hall (QAH) states that emerge in tMBG. In contrast to magnetically doped topological insulators, these QAH states are driven by intrinsic strong interactions, which polarize the electrons into a single moiré miniband with Chern number of C = 2. The magnetization of these “orbital Chern insulators” (OCI) arises predominantly from the orbital motion of the electrons rather than the electron spin. This orbital character of the magnetization allows one to control its magnitude and even change the sign by gate-tuning the chemical potential. Such curious magnetic properties of OCIs enable non-volatile electrical switching of the magnetic and topological orders [1, 2]. In addition to QAH states at integer fillings of the moiré superlattice unit cell, tMBG also features QAH states at half-integer fillings. These states are consistent with topological charge density wave states that partition a C=2 spin- and valley-polarized band into two C=1 sub-bands by spontaneous doubling of the superlattice unit cell [3].

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# Magnetic properties of moiré superlattice nanostructures

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Moiré superlattices formed by transition metal dichalcogenide (TMD) heterostructures are quantum simulators with highly tunable parameters. Several many-body interacting states of triangular lattice Hubbard model have been already observed like Mott insulator states and generalized Wigner crystal states. We investigate the magnetic properties of partially filled moiré energy bands using a combination of exact diagonalization methods and density matrix renormalization group (DMRG). We start from a continuum model and focus on electron-electron interactions for partially filled topmost valence band. We create maximally localized Wannier functions using the projection technique and derive effective Hubbard-like model. The magnetic properties of the ground state at particular fractional fillings are determined. We use DMRG to find the ground state properties of the effective spin models at the half-filling. Prospects for realization of exotic spin phases are discussed.

# SU(N)-Hubbard models and their simulations in cold atom and moiré systems

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The experimental realisation of multi-component SU(N)-Hubbard models using 173Yb or 87Sr atoms [1-3], with N > 2, has initiated a prolific cross-fertilization between the fields of quantum simulations and solid-state physics. More recently, twisted bi-layers of transition metal dichalcogenides (TMD) [4-5] have been shown to represent an ideal tunable platform for the realisation of multi-flavour correlated insulators [6].

In my talk, I will present theoretical calculations for the normal state of the SU(3)-Hubbard model in presence of a coupling between the different flavours, which is experimentally obtained via Raman coupling between hyperfine atomic levels. In particular, I will show how a real coupling leads to selective physics where different components of the fluid display different behaviours [7,8]. When the coupling becomes complex, it can be viewed as a hopping along the “synthetic” dimensions spanned by the flavour indices and induces chiral currents. I will discuss how such currents are strongly renormalised by correlation effects [9].

Finally, I will show a study of the SU(4)-Heisenberg model on a triangular lattice in presence of a field that splits the onsite energy of flavour pairs, which is believed to capture the salient features of AB-stacked twisted bilayers of WeSe2 in an electric displacement field. We display a phase diagram in the plane field vs next-neighbours-exchange including different symmetry-broken phases with simultaneous (anti-)ferromagnetic spin and excitonic order [10]. Furthermore, we demonstrate that there is a strongly fluctuating regime without long-range order that connects candidate spin liquids of the SU(2) and SU(4) limit. Our data also reproduce the strong layer polarizability which has been observed experimentally.

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# Understanding Excitations in Nano-antennas made from 2D-materials and Hybrid Systems

**Carsten Rockstuhl**[1], Marta Pelc[2], David Dams[1], Abhishek Ghosh[2], Miriam Kosik[2], Marvin M. Müller[1], Garnett Bryant[3], Andrés Ayuela[4], and Karolina Słowik[2]

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In this presentation, we explore the excitation dynamics in nano-antennas made from 2D-materials and hybrid systems thereof consisting of additional add-atoms, emphasizing the limitations of classical plasmonics in describing these phenomena. In our work, we exploit an efficient time-domain tight-binding framework to model the quantum optical interactions between nanoantennas and add-atoms, including chemical interactions. By studying model systems, such as polyene and polyacetylene molecules through the Su-Schrieffer-Heeger model, and more complex graphene nanostructures, we explore the intricacies of optical modes in these nanosystems. Our analysis reveals significant modifications in optical properties due to electronic tunneling between the add-atom and the nanoantenna, highlighting two distinct interaction regimes based on the add-atom's position. Furthermore, we propose an energy-based plasmonicity index (EPI) to redefine plasmon excitation, offering a novel perspective that aligns with energy-space coherence dynamics, providing a complementary approach to existing classifications and enhancing our understanding of plasmonicity in nanostructured materials.

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# Solid State, Atom-based Devices for Analog Quantum Simulation and Quantum Manipulation

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NIST is using atomically precise fabrication to make donor/quantum dot devices for individual electron manipulation and arrayed few-donor devices for analog quantum simulation (AQS). The goal of the AQS experiments is to explore the Hubbard phase space by fabricating atomically engineered materials whose properties, such as magnetic ordering or Mott insulating phase, depend on the detailed parameters of the atomic configurations. We are also studying donor/quantum dot devices to map out the energy spectrum and spin filling of single/few donor clusters, which form the basis of Hubbard arrays and prototype qubits. We use remote, high bandwidth RF reflectometry for charge sensing in arrays and individual spin measurements.

I will introduce the Hydrogen-based scanning probe lithography technique used for deterministic placement of individual dopant atoms and recent advances that enable fabrication with true atomic perfection. I will describe arrays of few-atom clusters we have fabricated in silicon that form the sites of a Hubbard model array in the strong interaction regime, where we vary the tunnel coupling from a weakly to strongly tunnel coupled regime. We map the Hamiltonian parameters to the physical system to tune the charge occupation, the spatial distribution of the eigenstates, localization/delocalization transition, and spin filling.

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# Gate screening of Coulomb interactions in Bernal bilayer graphene

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Gated bilayer graphene devices are subjected to a gate screening effect, wherein the Coulomb interactions within the bilayer are partly screened due to the electrostatic potential at the gates [3]. The amount of Coulomb interaction within the bilayer is thus expected to correlate with the strength of the gate screening effect. Therewith an influence of the gate screening strength on the formation of correlated states can be assumed.
We have investigated the influence of the gate induced Coulomb interaction screening on the appearance of previously reported correlated phases in gated Bernal bilayer graphene devices [1][2], using the thickness of the dielectric hBN spacing layers as variable parameter. In direct comparison with the data of Seiler et al. [1] we observed behaviour, which is supportive of an effectively lowered magnitude of Coulomb interactions in a sample using thinner hBN layers.
Additionally, three features in the transport data were identified, which could potentially be indicative of phases, not reported in [1] and [2].

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# Imaging quantum oscillations in strongly correlated moiré systems

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De Haas-van Alphen quantum oscillations in magnetization have traditionally served as the prime tool for determining the band structure of metals and semiconductors. Utilizing a scanning SQUID-on-tip, we image thermodynamic quantum oscillations with nanoscale spatial resolution and at very low magnetic fields, which allows reconstruction of the local band structure with high energy resolution. In Bernal-stacked trilayer graphene with dual gates, we reconstruct the band structure and its controllable evolution with the displacement field with unprecedented precision and map the naturally occurring strain-induced pseudomagnetic fields as low as 1 mT, corresponding to graphene twisting by 1 millidegree over 1 μm distance [1]. In Bernal bilayer graphene aligned to hBN, we reveal complex band structure with narrow moiré bands and multiple overlapping Fermi surfaces separated by very small momentum gaps. In addition to conventional oscillations obeying Onsager quantization, pronounced quantum oscillations are found to arise from particle-hole superposition states induced by coherent magnetic breakdown [2]. In twisted trilayer graphene, we observe renormalization of the single-particle band structure by Coulomb interactions greatly increasing the bandwidth of the flat bands and leading to symmetry breaking at half filling. On approaching charge neutrality, we find the ground state to be a nematic semimetal in which the flat-band Dirac cones migrate towards the mini-Brillouin zone center, spontaneously breaking the $C_3$ rotational symmetry.

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# Quantum Anomalous Hall Effect in Rhombohedral Graphene

**Presenter: Fan Zhang**

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The quantum anomalous Hall (QAH) effect is a robust macroscopic topological quantum phenomenon characterized by quantized Hall resistance at zero magnetic field. In this talk, I will first introduce the theoretical prediction of a family of QAH octets in interacting rhombohedral graphene systems [1]. Extraordinarily, for these QAH states, the Chern number aligns with the number of graphene layers. Furthermore, ferroelectricity, orbital magnetism, and band topology synergize to enable coexistence, facilitating switching within the octet via electric field, magnetic field, and carrier sign modulation. Next, I will highlight a recent experimental endeavor using suspended bilayer and trilayer devices [2,3], wherein the interaction effect is maximized allowing for the stabilization of QAH octet at small fields, as well as a more recent experimental breakthrough: the observation of the fully quantized QAH effect at zero magnetic field in a h-BN encapsulated, WS2 proximitized, pentalayer device [4]. Finally, I will discuss the roles played by WS2 and if time permits, other exotic correlated physics in rhombohedral graphene systems, such as the fractional QAH states.

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# Exploiting Crystal Lattice for Efficient, Atomistic Computations of Multi-Million Atom Nanostructures

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Theoretical understanding of spectra of typical nanostructures is often far too challenging for ab-into approaches. In contrast, non-atomistic approaches fail to explain their spectra' crucial details. On the other hand, atomistic approaches can adequately handle essential spectra features at a moderate computational cost. Here, I discuss our recent progress [1-5] in atomistic modeling of a broad range of nanostructures. We exploit the properties of the underlying crystal lattice and run calculations on a regular three-dimensional grid superimposed on the original, lower-symmetry lattice [1,2]. This allows linear scaling of (quasi)particle interactions with multi-million atom calculations to be performed within several minutes. Moreover, we demonstrate that the same computational tools can simulate the whole zoo of systems, from alloyed and crystal phase quantum dots up to lattices of dopants in silicon [1-5].

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# Contributed talks

# Exploring the Magnetic World of transition metal Ilmenenes

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Iron ilmenene, a novel two-dimensional material recently extracted from naturally occurring iron titanate in ilmenite ore, is the focus of our investigation. We aim to comprehensively analyse the structural, electronic, and magnetic properties of 2D transition metal-based ilmenene-like titanates. Our examination of magnetic ordering reveals a consistent intrinsic antiferromagnetic coupling between the 3d magnetic metals decorating both sides of the Ti-O layer within these ilmenenes. Through calculations incorporating spin-orbit coupling, we uncover significant magnetocrystalline anisotropy energies in magnetic ilmenenes, particularly when the 3d shell deviates from full or half-filled occupancy. Notably, the spin orientation tends to align out-of-plane for elements below half-filling of 3d states and in-plane above. These fascinating magnetic properties underscore the potential of ilmenenes for future spintronic applications, building upon the successful synthesis observed with iron counterparts.

# Ferromagnetic order in 2D layers of transition metal dichlorides

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Metal dihalides (TMDH) are a class of 2D layered materials bonded through van der Waals interactions. These binary compounds exhibit magnetic texture with semiconducting electronic properties. Since single layers can grow epitaxially on metal substrates, there is a strong interest in determining whether these properties persist at the 2D limit [1-3].

Here we study the epitaxial growth of $FeCl_2$ and $NiCl_2$ on Au (111). Their chemical and electronic properties were explored high-resolution X-ray photoelectron spectroscopy (XPS) and low-temperature scanning tunneling microscopy and spectroscopy (STM). These 2D materials grow in large and flat monolayers electronically decoupled from the substrate. Our studies on the magnetic properties by X-ray absorption spectroscopy (XAS) revealed a ferromagnetic order related to the 3d electrons of the metal in the compound. The magnetic alignment depends on the TM used, so that it can be switched from out-of-plane to in-plane by substituting the metal ion from iron to nickel. Furthermore, we investigated and established a correlation between the mesoscopic magnetic properties and the atomic spins utilizing STM tips functionalized with nickelocene.

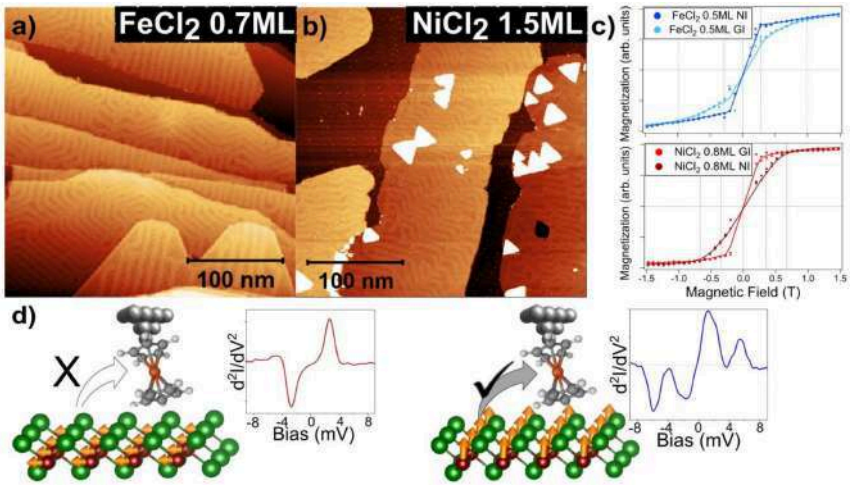


**Fig 1.** (a-b) STM constant current images of the first layer of $FeCl_2$ and $NiCl_2$ on Au (111) respectively. (a) I=20pA U=3.0V b) I=10pA U=2.0V). (c) Comparison of magnetization loops for $FeCl_2$ and $NiCl_2$ at normal (NI) and grazing incidence (GI) measured at the Fe (c) and Ni (d) $L_3$ edge. d) Nickelocene (Nc) STM tip-decorated measurements on monolayers of TMDH.

If the magnetization axis of the adlayer is parallel to that in the Nc, it is sensed as a splitting in the inelastic electron tunneling spectroscopy curves.

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# Coupling between single emitters and plasmonic nanoantennas: Quantum effects revealed by time-dependent density functional theory

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# Bloch spectroscopy of graphene superlattices and applications in photon detection

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Moiré quantum materials present exciting prospects for fundamental physics, owing to the delicate interplay between long-range superlattice effects and inter-band hybridisation. Our study focuses on the superlattice formed when bilayer graphene is aligned with hBN in which a slight lattice mismatch gives rise to a periodic moiré potential acting on charge carriers and leading to the formation of Bloch mini bands.

We found a regime of negative differential conductance when the superlattice is subject to an electric field large enough to shift the Fermi surface out of equilibrium and trigger Schwinger-like electron-hole pair creation. We mapped out the electronic band structure of bilayer graphene superlattices using high-bias features. We propose optoelectronic devices harnessing this negative differential conductance, including bolometers with broadband functionality and single photon detectors. Our findings suggest that bilayer graphene superlattices are promising for exploring Bloch oscillations and hold significant potential for the development of novel optoelectronic devices.

# Non-empirical prediction of electronic and optical properties of van der Waals materials from a Wannier-localized optimally tuned screened range-separated hybrid functional

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There is wide interest in the electronic and optical properties of van der Waals (vdW) materials. Accurately predicting these properties with density functional theory, however, has been difficult. Wannier-localized, optimally tuned, screened range-separated hybrid (WOT-SRSH) functionals [1] have been used successfully for determining the electronic band gaps and optical absorption spectra of a variety of materials [1-3]. However, for vdW materials only semi-empirical approaches have been used, to date, to tune the material- and structure-dependent functional parameters [4, 5]. Here, we develop and apply a fully non-empirical WOT-SRSH approach for determining the functional parameters and we show, using several prototypical vdW materials, that this approach yields a level of accuracy comparable to that of ab initio many-body perturbation theory.

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# Enhanced and Tunable Spin-Orbit Coupling in Bilayer Graphene/Transition-Metal Dichalcogenide Quantum Devices

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We characterize quantum point contacts and quantum dots in bilayer graphene/transition-metal dichalcogenide (TMD) heterostructures across multiple devices using both WSe2 and MoS2 as the TMD layer. In contrast to pristine bilayer graphene, where the intrinsic spin-orbit coupling (SOC) ranges typically from 40-80 μeV [1,2], we measure enhanced values of up to 1.4 meV by adding TMD to the heterostructure. Moreover, we demonstrate the tunability of the SOC strength from its maximal value to complete suppression through manipulation of the perpendicular electric field. This increased SOC strength combined with its tunability holds great potential for future quantum computing and spintronics applications. As a high SOC is beneficial for the fast driving of qubits, integrating bilayer graphene with TMD presents a promising platform for realizing qubits in 2D systems.

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# Unconventional magnetic properties of epitaxially grown 2D Semiconductor FeBr2 grown on Au(111)

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Over the last years the research on magnetic two-dimensional materials has increased constantly by focusing more on the precise control of thickness down to the single-layer limit. A promising candidate for 2D magnetism is FeBr2. Here the structural characterization was performed via LT- STM and LEED, which revealed a dominant superstructure of the strained first layer. By increasing the coverage above the ML-limit, the superstructure disappears and the non-strained FeBr2 lattice can be observed. The XPS and XAS measurements revealed that the chemical composition does not change for increasing coverages. However, by comparing the magnetic properties of the ML sample with the multilayer film strong differences in the measured saturation magnetization as well as magnetization behavior has been observed. Additionally performed linear dichroism measurements revealed a strong structural change for the different coverages, which underlined the obtained LEED and STM results.

# Nonlinear optical phenomena in 2D-like materials

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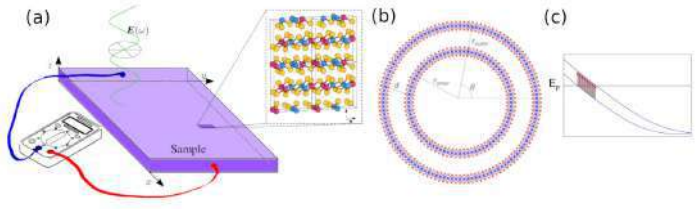
Recently a focus of renewed attention, the bulk photovoltaic effect (BPE) is a nonlinear absorption phenomenon that converts light into electrical current intrinsically [1]. While traditionally it has been mostly studied in bulk ferroelectrics, recent works have emphasized that it undergoes a significant enhancement in 2D systems [3, 4] with strong links to topology [5].
In this contribution, we discuss the BPE combining the predictions of our theoretical approach based on Wannier interpolation [6] with recent optical measurements in several types of 2D-like materials and structures like TMD nanotubes, layered Weyl semimetals and Rashba surface states (see figure). These offer an ideal bridge between a purely 2D system and a bulk crystal structure, and exhibit accutely enhanced nonlinear light-absorption capabilities [3, 7]. Elucidating the microscopic origin of the underlying physical mechanisms often requires accounting for nontrivial responses such as third-order effects [8].

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# Photogalvanic effects in twisted bilayer graphene

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The chiral lattice structure of twisted bilayer graphene allows for intrinsic photogalvanic effects only at off-normal incidence which have been neither computed nor measured so far. In this work, we first compute the intrinsic effects and show they reverse sign at the magic angle, revealing a band inversion at the Brillouin Zone origin. We next consider different extrinsic effects induced by a substrate or a gate potential, showing how they can be used to track the strengths of the substrate coupling or displacement field. We also show that an approximate particle-hole symmetry implies stringent constraints on the chemical potential dependence of all photocurrents. A detailed comparison of intrinsic vs. extrinsic photocurrents therefore reveals a wealth of information about the band structure and can also serve as a benchmark to constrain the symmetry breaking patterns of correlated states.

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# Robustness of type-II Dirac cones in biphenylene-based structures

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Inspired by the discovery of graphene's unique properties due to its geometry [1], researchers have explored new 2D materials like graphynes [3], graphydyine [4], and others. Merging graphene with other geometries has led to exciting discoveries, such as the recently synthesized biphenylene [2]. Composed solely of carbon atoms with sp2 hybridization in hexagonal and square arrangements, biphenylene attracts attention for its metallic 2D properties, including a type-II Dirac cone and semiconducting character in small armchair nanoribbons. This work explores the electronic properties and symmetries of bipheny- lene in van der Waals heterostructures with several stacking configurations. We employed an exponential hopping tight-binding model with several neighboring sites able to capture the type-II Dirac cone, pre- dicted by density functional theory calculations. The robustness of the type-II cones was observed in various configurations, from bilayers to nanoribbon biphenylene systems. Transport calculations were performed using the TB model parameters with the Landauer-Buttiker formula and Green's function formalism.

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# Straintronics and adatoms to enhace and tune the magnetic response in graphene nanoribbons

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The possibility that a non-magnetic material such as graphene could exhibit magnetism stemming from pz orbitals has attracted the attention of researchers for more than a decade. Graphene nanoribbons with zigzag edges are regarded as one of the most intriguing systems for investigation. Theoretically, unlike bulk graphene, they are anticipated to display intrinsic magnetism due to the spin polarization of their edge states, making them ideal for spintronics. However, the detection of this edge magnetism remains challenging, as structural defects at the edges of synthesized ribbons appear to dampen the magnetic response, a phenomenon highly sensitive to the atomic precision of the edges.

In this work we present the possibility of increasing the magnetic response of zigzag graphene nanoribbons by applying strain in the longitudinal direction of the ribbon. This could facilitate the experimental detection of magnetism. We perform DFT calculations, which are compared with a tight-binding Hubbard Model in mean field approximation, that allows great versatility and scalability of the calculations. Both models fit together with remarkable precision. As a result of the modification of the bands, increases in magnetization close to 90% are obtained at strain values of 15%. We also study the possibilities of modifying magnetism through the selective deposition of hydrogen adatoms, combined with strain. These are already experimentally handled with atomic precision in graphene and can also help to better understand the magnetic dependence on defects.

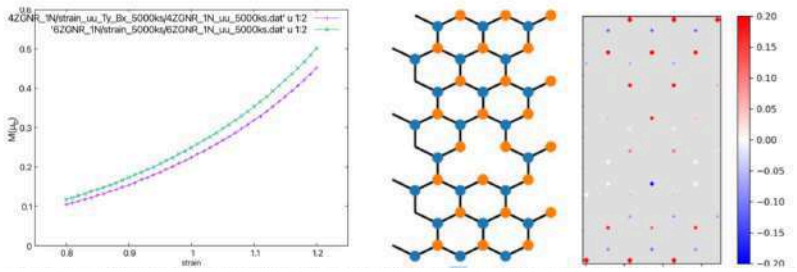

**Figure 1:** Left: Magnetic moment of an edge atom as a function of strain. Center: system with a vacancy and a 15% of applied strain. Right: Resultant magnetization from the previous system

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# Superexchange Mechansim in Coupled Triangulene Chains

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One-dimensional chain of spins S = 1 reveal symmetry-protected topological order with a gapped excitation spectrum in a periodic system, called the Haldane gap, and characteristic spin S=1/2 edge excitations, when the system is finite [1]. Various ways exist to create physical realizations of spin chains, for example using the scanning tunneling microscope (STM) on solid surfaces by manipulating molecules with atomic precision [4]. Recently, a chain of triangulenes [5], a 22-Carbon atom triangular graphene quantum dot with zigzag edges revealed features of an $S$ = 1 spin chain [6]. This is related to the fact that a single triangulene molecule has a ground state with total spin S=1, in accordance with Lieb's theorem on a Hubbard model [7] and the fact that neighboring triangulenes are coupled antiferromagnetically.

Here we show that the antiferromagnetic coupling in spin-1 triangulene chains originates from a superexchange mechanism. This process, mediated by inter-triangulene states, opens the possibility to control parameters in the effective bilinear-biquadratic spin model. Using a combination of tight-binding, Hartree-Fock, density functional theory and configuration- interaction we obtain the low-energy many-body spectrum for $N$!" = 2 and $N$!" = 4 triangulene and show that it agrees with the bilinear-biquadratic spin-1 chain antiferromagnetic model when indirect coupling processes, and superexchange coupling between triangulene spins are taken into account [8].

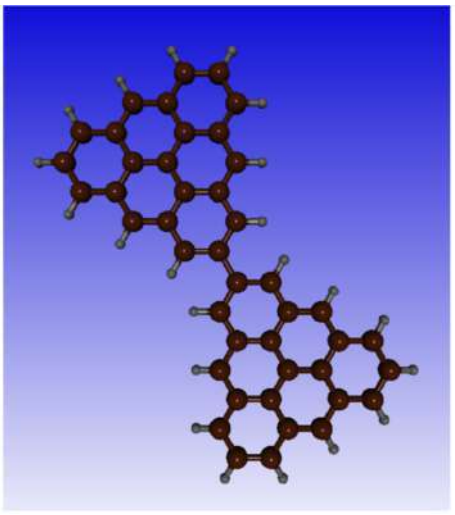

Figure 1 – Antiferromagnetically coupled trianguelene molecules.

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# Quantum Geometry and Stabilization of Fractional Chern Insulators Far from the Ideal Limit

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In the presence of strong electronic interactions, a partially filled Chern band may stabilize a fractional Chern insulator (FCI) state, the zero-field analogue of the fractional quantum Hall phase. While the FCI phase has been long hypothesized, feasible solid-state realizations only recently emerged, largely due to the rise of moire´ materials. In these systems, the quantum geometry of the electronic bands plays a critical role in stabilizing the FCI over competing correlated phases. Whereas in the limit of “ideal” quantum geometry this role is well under- stood, only empiric numerical evidence exist away from ideal conditions, without clear analytical understanding of how the FCI deteriorates. We analyze an anisotropic model of a |C| = 1 Chern insulator, whereupon partial filling of its bands, an FCI phase is stabilized over a certain parameter regime. We incorporate strong electronic interaction analytically by employing a coupled-wires approach, analyzing the FCI stability, and its relation to a parameter which controls the quantum metric. We identify an unusual anti-FCI phase benefiting from non-ideal geometry, generically subdominant to the FCI, however its presence hinders the FCI formation in favor of other phases. We thus establish an analytical connection between quantum geometry and FCI stability far from any ideal band conditions.

# Pathway to Quasi-2D Time Crystals Using NISQ Hardware

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Recent advancements have showcased the capability of noisy intermediate-scale quantum (NISQ) hardware to create many-body localization using a one-dimensional chain of spins, subjected to periodic driving [1-5]. These implementations reveal several useful features, including period multiplicity under periodic driving, retention of initial state information amidst noise, and other characteristics indicative of a phase of matter known as a discrete time crystal (DTC). However, these demonstrations have primarily been confined to one-dimensional systems. It has been suggested that the distinctive traits of a DTC might extend to two-dimensional and quasi-two-dimensional lattice structures [6]. The pathway to implementing these structures on cutting-edge NISQ hardware (e.g., IBM Torino), at a scale that cannot be simulated classically, possesses several challenges, including error correction and mitigation. We demonstrate this pathway by simulating the dynamics of a quasi-two-dimensional heavy-hexagonal spin ½ lattice on 125 qubits. We address the intricacies associated with implementation of these lattices on NISQ devices, the challenges posed by such a scale, and outline avenues for further exploration into the characteristic signatures of many-body localization.

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# Posters

# Quantum effects in the optoelectronic coupling between plasmonic nanoantennas and single emitters

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In this work, we theoretically explore the optoelectronic response of plasmonic nanoantennas coupled to single emitters via plasmon--exciton interaction (see Figure 1). Focusing on nanometer-scale systems, our investigation considers nonlocality, nonlinearity, and electron-transfer processes, which are crucial factors in understanding these complex interactions. To analyze all these phenomena, we primarily use Time-Dependent Density Functional Theory (TDDFT) and complement the study using a semiclassical model referred to as the Surface-Response Formalism (SRF). The SRF accounts for quantum surface effects through the inclusion of the Feibelman parameters in the boundary conditions of Maxwell's equations.
Our findings reveal that electron spill-out and surface-enabled Landau damping exert a profound influence on the electromagnetic interaction between plasmonic nanoantennas and single emitters at the nanometer scale. This influence results in a redshift and broadening of plasmonic resonances, phenomena not captured by classical theories [1]. We demonstrate that the semiclassical SRF, particularly when considering the nonlocality of the response in the direction parallel to the metal surface, accurately describes these effects [2].
Furthermore, our study predicts that the hybridization between electronic states of emitters and plasmonic nanoantennas significantly impacts the optical response of the coupled system at subnanometric distances [3]. The electronic transition in the single emitter is entirely quenched due to this electronic exciton-plasmon coupling, dramatically altering the frequency and width of the optical resonances sustained by the coupled structure and hindering the strong exciton-plasmon coupling.
Finally, we showcase that the electromagnetic coupling of an emitter to a spherical plasmonic nanoantenna can induce notable changes in the nonlinear optical response, unlocking otherwise-forbidden second harmonic generation (SHG) [4]. Overall, these findings deepen our fundamental understanding of quantum phenomena in nanoscale plasmon–exciton interactions.

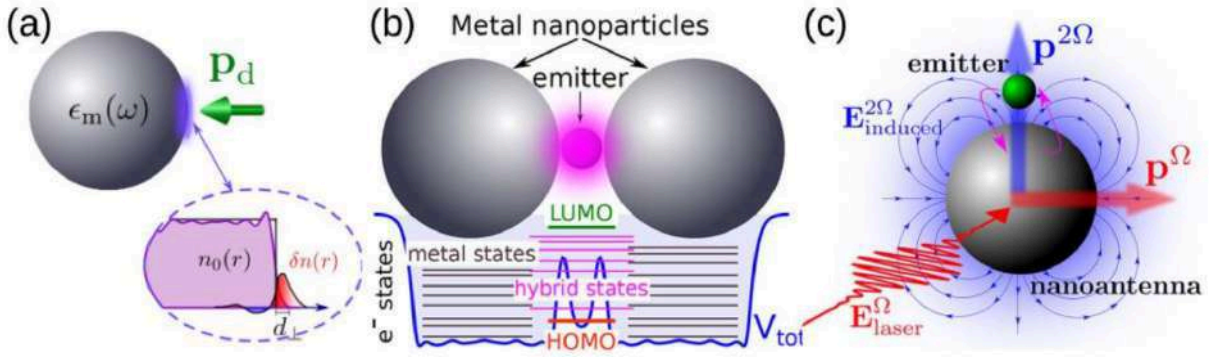


Figure 1: Sketch of the studied systems: (a) Quantum surface effects in the electromagnetic interaction between a spherical plasmonic nanoantenna and a single emitter. (b) Electronic coupling and charge-transfer effects in plasmon-exciton coupling in a metallic nanocavity. (c) Second-harmonic generation from a single emitter coupled to a spherical plasmonic nanoantenna.

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# Effects of Vacancy Defects on the Transport Properties of 2D $Mo_2ScC_2O_2$

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The impact of vacancy defects on the transport properties of the 2D $Mo_2ScC_2O_2$ monolayer was investigated using density functional theory in combination with the non-equilibrium Green's function method. It was found that defects are location-independent on the surface and that O vacancies are energetically more favorable than Mo vacancies. Only Mo divacancies produced a magnetic moment. Furthermore, the research demonstrated that defects on the 2D $Mo_2ScC_2O_2$ do not compromise its metallic character or significantly affect its electronic transport properties.

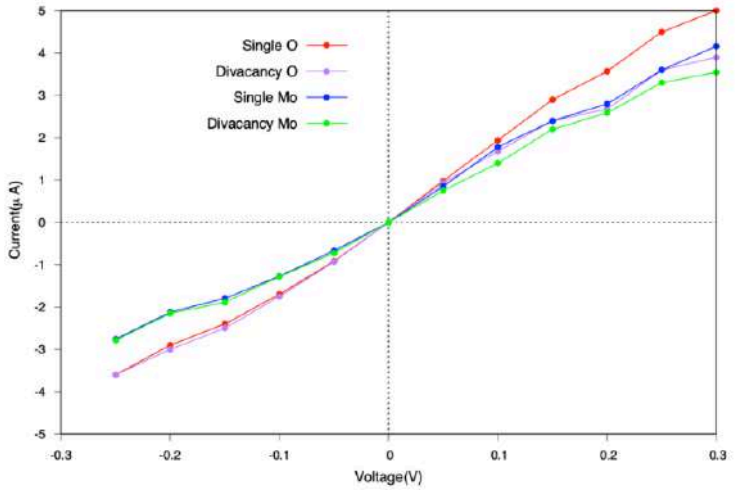


Figure 1: I-V Characteristic for defective devices.

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# Light-matter interaction effects at the carbon nanoscale

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Carbon-based structures such as graphene or polyacetylene chains have played an important role at the forefront of condensed matter research, paving the way for new practical applications and theoretical insights. Harnessing their potential for light-matter applications and plasmonics, however, is still an actively researched question. We discuss a theoretical and computational description of light-matter interactions in nanoscopic carbon allotropes, allowing for a real-space description of light-matter interaction effects at the nanoscale.

# GRANAD: GRAphene Nanoantennas with ADatoms toolbox

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Understanding the optoelectronic properties of mesoscopic graphene nanoflakes and one-dimensional polymer chains with adatom defects presents significant conceptual and computational challenges. Traditional methods, including commercially available software, may lack the capability to capture quantum effects at this scale, while ab initio quantum mechanical approaches are computationally demanding. To address this gap, we introduce GRANAD: the GRAphene Nanoantennas with ADatoms toolbox, an open-source software package.
GRANAD employs the tight-binding approximation to model the underlying matter and treats light semiclassically. With a focus on mesoscopic systems, GRANAD utilizes a single electron mean-field method for many-body systems, where interactions are mediated through non-linearities in the Hamiltonian [1,2] . It evolves the system using a Lindblad-like master equation for the spin-traced one-particle reduced density matrix, incorporating dissipative processes within the master equation. This approach allows GRANAD to calculate various static quantities such as the energy landscape, density of states, absorption spectra, and dynamic quantities like induced dipole moment and energy-based plasmonicity index (EPI) [3].
GRANAD's foundational implementation relies on conventional Python-based object-oriented programming. However, its core functions are crafted using the functional programming paradigm with GOOGLE's JAX library, enabling an auto-differentiation feature. This functionality, for instance, allows for automatic electric field optimization to elicit a desired response from a nanostructure. Moreover, this JAX implementation demonstrates significantly faster performance on GPU compared to conventional CPU implementations.

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# Polar quantum systems in the vicinity of nanoparticles

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This study explores a widely used model that approximates the quantum system with two energy levels. The optical characteristics of this model are determined by spatial symmetries, characterized by multipolar transition moments. When subject to a resonant plane wave, the system undergoes cyclic population transfers between its levels, commonly referred to as Rabi oscillations. In the simplest scenario, the frequency of these oscillations scales linearly with the amplitude of the driving field and the transition dipole moment of the quantum system.

Our investigation extends beyond conventional analyses by incorporating polarity into the model. This means the system exhibits distinct permanent dipole moments in its ground and excited states, introducing an extra oscillating dipole during population transitions [1]. This modification significantly alters the system's response to the driving field, leading to profound implications such as the emission of low-frequency radiation [2], and nonlinear corrections to both the Rabi frequency and spontaneous emission rate, concerning the amplitude of the driving field. Surprisingly, these aspects have not been extensively explored in existing literature.

Due to these properties, it is particularly interesting to investigate the dynamics of polar systems in the vicinity of nanoparticles. Their well-known features, such as enhancement of the spontaneous emission rate of coupled systems, and confinement of incident light, provide an ideal environment for studying the nonlinear behavior of polar systems. We especially demonstrate that the nonlinearity of the Rabi frequency can improve the coherence of the collective response of multiple systems driven in a strongly space-varying field.

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# Spin-Momentum Locked Defected Bilayer Graphene

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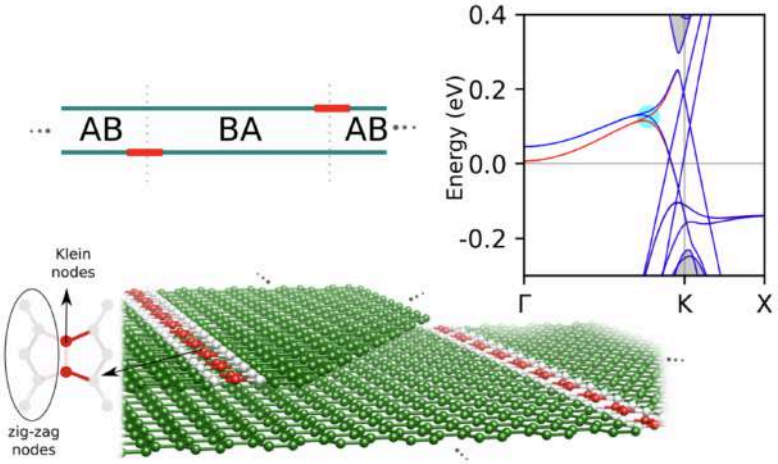
Graphene few-layer structures still presenting exciting phenomena to discover. For instance, studies on twisted bilayer graphene (BLG) show superconductivity [1], a fact that has expanded research on the stacking of few layer graphenes [2]. Different phenomena can be achieved by including domain walls in the bilayer graphene and thus causing the change from AB to BA stacking [3-4]. In fact, pentagons and octagons (8-55) defect lines, see Fig. 1, can achieve such purpose and induce topological states in the bulk gap. These defect lines can induce states that correlate with topological ones around the band gap [5,6]. In this work, using density functional theory calculations, we investigate an array of these defect lines in BLG. We found that the band structure shows a magnetic phase in which the spin is locked to the momentum, as in topological insulators. We also follow the topological states that appear even without a gate because of the array of defect lines. We lastly study the differences in spin bands and identified topological states when engineering by doping and/or electric field. All these results are summing to the new interesting data of the correlated behaviour of electrons with the stacking in two-dimensional materials.

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# Ultra-Narrow Resonance and High-Q Factor in Hexagonal Boron Nitride Metasurface for Enhanced Many-Body Interactions in the Visible Regime

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This study presents investigation of the properties of complementary hexagonal boron nitride (h-BN) metasurface. This h-BN metasurface has a hBN layer 150 nm thick with an elliptical hole, sitting on a SiO2 layer. The structure sustains ultra-narrow resonances over the complete visible spectrum, with a high Q-factor exceeding 75,000. The achieved resonance bandwidths are smaller than 0.007 THz, while the electric field enhancement surpasses 250. The proposed h-BN metasurface design facilitates coherent light-matter interactions within a large volume.It can operate within the challenging constraints of the visible spectrum, thus marking a significant step in manipulating light-matter interactions at the nanoscale, potentially opening new avenues for research and applications in the field[1, 2].

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# 2D-like Frenkel Excitons in the Calcite Polymorph of $CaCO_3$

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Calcite(CaCO3) belongs to the materials with intriguing optical properties to be present in radiative cooling applications [1], being one of the main constituents of limestone that serves as the primary source for cement production [2]. Despite its broad industrial and geological relevance, the optical characteristics of calcite remain relatively understudied.
Room temperature X-ray diffraction experiments on calcite agree upon a=b=4.99 Å and c=17.06 Å lattice parameters [3]. Calcite has the Ca cations occupying pseudo-cubic lattice sites with an octahedral environment formed by oxygen atoms. The CO3 groups with trigonal symmetry are located at the vertices of Ca octahedra, giving rise to a planar arrangement. Furthermore, CaCO3 polymorphs are well-known for their significant birefringence, attributed to the planar arrangement of CO3 groups perpendicular to the crystallographic z plane. Several experimental works have also reported a strong prevalence of reflectance within the CO3 plane (ordinary ray), with peaks observed at 7.55 eV and 7.75 eV [4], whereas a single peak at 8 eV is present in ref. [5]. Kondo et al. explained the main spectral feature as a localized molecular excitation of the CaCO3 radical. Despite its technological importance, the optical properties of CaCO3 has not been extensively studied.

In this work we present the optical properties of CaCO3 calcite, obtained through first-principles methods. We use density functional theory (DFT) with the SCAN meta-GGA [6] approximation for the exchange-correlation functional. For the optical spectra calculations, the band structure was refined using GW many-body perturbation theory [7], and the electron-hole interactions were modeled by solving the Bethe-Salpeter Equation (BSE) [7]. The inclusion of electron-hole interactions in BSE redistributes spectral weights to lower energies, causing a red-shifts of the GW spectrum.

The position of the main spectral peak aligns perfectly with experimental observations. Our findings indicate that the onset of the CaCO3 optical spectrum is characterized by a bound exciton, which shows significant 2D-like anisotropy and the localization of the excitonic wave function on the CO3 units. Given its large binding energy spacial extent, we conclude that the exciton is Frenkel molecular-type. This insight underscores the material unique excitonic behavior and its implications for optical applications.

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# Tuning the magnetic properties of layered materials through organic ion intercalation

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Intercalation is the insertion of guest species in the van der Waals gap of a host layered material. The process is accompanied by a significant change in the material's charge carrier density and in its interlayer distance, overall yielding a profound modification of its band structure. The intercalation of organic molecules offers multiple options to tailor the physical properties of layered materials due to their very different size, charge, electrical dipole, magnetic spin and optical properties.

Here, we report on the tuning of the magnetic properties of antiferromagnetic $MnPS_3$ through the intercalation of organic ions. In particular, $MnPS_3$ was intercalated with four alkylammonium bromide salts ($R_4NBr$, with $R_4$ = tetramethyl, tetraethyl, tetrabutyl, cetyltrimethyl) in aqueous solutions. X-ray diffraction, Raman, and gravimetric studies were carried out for structural characterizations of the intercalated compounds. Magnetometry measurements revealed that while pristine $MnPS_3$ are antiferromagnets, the intercalation of organic ions introduces a molecule-dependent ferrimagnetic response, which remains down to the few-layer thickness. The four $R_4N$-$MnPS_3$ intercalates ($T_C$ ~ 45-55 K) display a hysteresis loop with saturation magnetization reaching up almost 1 $\mu_B$/atom. Our results establish organic ion intercalation as an effective tool to control the magnetism of layered magnetic materials.

# Nanoscale Charge Transport Characterization of Novel Type 2D MOFs

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In recent years, Metal Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) have emerged as fascinating and promising materials classes, owing to their exceptional structural versatility and tunable properties, which make them interesting for a wide range of technological applications . At the same time, the study of 2D van der Waals materials has become the proba- bly most relevant and dynamic area in solid state research at present, offer- ing numerous opportunities to uncover novel physical phenomena and engineer advanced nanoscale devices. With recent advances in the synthesis of two-dimensional MOFs and COFs, these material classes have also entered the field of van der Waals materials. We will characterize the charge transport in novel type 2D coordination network materials like CuBHT, considering also the in- fluence of properties like structure or defects. By that, we will demonstrate why they are promising candidates for implementation into van der Waals het- erostructures and will further put a focus on quantum transport measurements on CuBHT.

# Towards magnetotransport measurements in rhombohedral penta-layer graphene

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Graphene is one of the most studied 2D material to-date. Due to its band structure, rhombohedrally stacked multi-layer graphene has been the subject of recent studies. Notably the discovery of superconductivity in tri-layer graphene attracted significant attention [1]. Penta-layer graphene is currently of particular interest for the study of electron correlation effects due to its high density of state stemming from increased flat bands near the band edge [2, 3]. This work shows how rhombohedrally stacked regions of mechanically exfoliated penta-layer graphene can be identified via Raman spectroscopy and spatially resolved in the nanometer regime by scanning near field optical microscopy (SNOM). Furthermore, a nanolithography technique to isolate such regions using an atomic force microscope (AFM) is presented, as well as the fabrication steps of hexagonal Boron Nitride (hBN) encapsulated dual gated magnetotransport devices and the stability of the rhombohedral stacking order during the fabrication process. Additionally, an outlook on the upcoming magnetotransport measurements in the milli Kelvin regime is discussed.

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