Novel electronic properties of two dimensional materials (NEP2DM)

July 11-15th San Sebastian, Spain

Poster booklet

Ahmed Abouelkomsan

Stockholm University

Moiré Superlattices at Fractional Band Fillings: Fractional Chern Insulators, Particle-Hole duality, and Quantum Geometry

We consider the core problem of Coulomb interactions within fractionally filled Moiré flat bands and demonstrate that the dual description in terms of holes, which acquires a non-trivial hole-dispersion, provides key physical intuition and enables more understanding for this strongly correlated problem. We find that the single-hole dispersion has a profound impact on the phase diagram in experimentally relevant examples such as ABC stacked trilayer and twisted bilayer graphene aligned with boron nitride. Such non-trivial particle-hole asymmetry which is generally absent in continuum Landau levels stems from the non-trivial underlying quantum geometry of the Moiré bands. In addition, we predict both twisted bilayer graphene aligned with boron nitride and gate-tunable twisted double bilayer graphene to be versatile platforms for the realization of fractional Chern insulator states like spin-singlet Halperin states and spin-polarized states in bands with Chern number $C = 1$ and $C = 2$ at zero external magnetic fields.

Mohammed M. Al Ezzi

National University of Singapore

Asymmetric correlated states in twisted monolayer-bilayer graphene

In twisted monolayer-bilayer graphene massless and massive Dirac fermions mix together and lead to asymmetric correlated states and out-of-equilibrium criticalities characterized by superconductivity-like non-linear current-voltage characteristics. In this theoretical work, we first develop an analytical model to explain the observed asymmetry in formation of correlated states with respect to carrier density and displacement field [1]. Using the linearized gap equation method, we calculate the stability and critical temperature for different symmetry breaking phases, including spin density waves, charge density waves, and valley ordered phases. We compare our theoretical findings with available experimental data.

[1] Shuigang Xu, et al. Nature Physics, 5 (2021)

Ivan Amelio

ETH Zurich

Polaron spectroscopy of the bilayer excitonic insulator

We study theoretically the polaron spectrum of an interlayer excitonic insulator (EXI) for different interlayer distances. First, the binding energy of the relevant few-body bound states is computed by Quantum Monte Carlo. In particular, we show that a ground state interlayer exciton can bind to a probe intralayer exciton (X-IX). Then, we describe the EXI in terms of BCS theory and study the polaron problem within a Chevy-like ansatz involving excited Bogoliubon pairs. Crucially, keeping interactions between Bogoliubons allows us to recover the X-IX feature as well as a trion line. Our predictions provide clear hallmarks of pairing in view of forthcoming experiments in bilayer systems, as well as general theoretical insights on polaron physics on top of paired phases.

David Barcons Ruiz

ICFO

Novel approach for graphene artificial superlattices: sub-20 nm period lattices and electron-hole symmetry breaking

The first observation of Hofstadter butterflies in graphene Moiré superlattices [1], and more recently, the discovery of superconductivity in MATBG[2], has attracted the community towards the study of these systems. Even though Moiré superlattices show very interesting phenomena, they lack basic tuning knobs, namely lattice symmetry and potential strength. Several groups have put effort in pushing nanofabrication techniques to engineer artifical graphene superlattices, but periods below 40 nm remain challenging [3-4].

We develop a new nanopatterning technique able to achieve sub-20 nm period lattices. Our technique combines He focused ion beam (FIB) indirect milling of suspended membranes with reactive ion etching (RIE), achieving ultimate FIB resolution and damage free patterning.

Employing this technique, we create artificial superlattices down to 18 nm period, approaching the lengthscales in MATBG.

Also, by engineering a non-bipartite superlattice (a Kagomé superlattice in our case), we demonstrate for the first time electron-hole symmetry breaking in single layer graphene.

Our technique opens the path to engineer exotic phenomena in single layer graphene, with symmetries not accessible in Moiré superlattices and dimensions well below the state of the art in nanofabrication.

[1] Ponomarenko, L. A., et al. Nature, 497.7451, 594-597, (2013)

[2] Cao, Yuan, et al. Nature 556.7699, 43-50, (2018)

[3] Forsythe, Carlos, et al., Nature nanotechnology, 13.7, 566-571, (2018)

[4] Huber, Robin, et al., Nano letters 20.11, 8046-8052, (2020)

Sergi Batlle Porro

ICFO

Photocurrent nanoscopy as a tool to investigate local twist angle and electron-hole asymmetry inhomogeneity in twisted bilayer graphene

The unexpected demonstration of superconductivity in magic angle twisted bilayer graphene [1,2] opened a new rapidly growing subfield of condensed matter physics. Moiré materials with their large superlattice unit cells offer to explore strongly correlated phenomena at very low charge carrier densities [1-6].

Current advances in scanning probe techniques have allowed the researchers to determine local properties of matter down to the size of sub-nanometer. In particular, scattering type scanning near-field optical microscopy (s-SNOM) is an ideal tool to explore MATBG [7,8] since it allows us to measure scattering and photocurrent signals at the nanometer scale while simultaneously probing mesoscopic electron transport through the sample [8-10].

With energies in the mid-infrared (MIR), we use a novel cryo-SNOM technique that allows us to perform s-SNOM at cryogenic temperatures (down to 10 K) and measure optical and photocurrent near-field response [10]. By back gate gate and temperature tunning, we can determine a twist angle map around 1.38±0.05° homogeneity and image correlated phenomena. Here we report how this photocurrent is related to the Seebeck coefficient through the photothermoelectric effect and how to extract twist angle, Drude weight and electron-hole asymmetry from local measurements. We observe Seebeck and Drude weight electron-hole asymmetry peaking for fillings between 2-3 and disappearing with increasing temperature. This work constitutes further proof of the role of electron-electron interactions play in twisted bilayer graphene samples and how it influences thermoelectric properties even far away from the magic angle.

[1] Yuan Cao et al. Nature 2018 556:7699, 556(7699):80–84, 2018.
[2] Yuan Cao et al. Nature 2018 556:7699, 556(7699):43–50, 2018.
[3] Xiaobo Lu et al. Nature 2019 574:7780, 574(7780):653–657, 2019.
[4] Petr Stepanov et al. Nature 2020 583:7816, 583(7816):375–378, 2020.
[5] Peter Rickhaus et al. Science, 373(6560):1257–1260, 2021.
[6] Ming Xie and A. H. Macdonald. Physical Review Letters, 124(9): 097601, 2020.
[7] Antoine Reserbat-Plantey et al. ACS Photonics, 8(1):85–101, 2021.
[8] S. S. Sunku et al. Science, 362(6419):1153–1156, 2018.
[9] Achim Woessner et al. Nature Communications 2016 7:1, 7(1):1–7, 2016.
[10] Niels C.H. Hesp et al. Nature Communications 2021 12:1, 12(1):1–8, 2021.

Raúl Bombín

Universitat Politècnica de Catalunya / Centro de Física de Materiales (Donostia)

Adsorption and dissociation of diatomic molecules on monolayer 1H_MoSe2

Two-dimensional transition-metal dichalcogenides appear as good candidates for gas sensing and catalysis. Here, by means of density functional theory, we characterize the adsorption and dissociation of selected diatomic molecules (CO, H2, O2, and NO) on the MoSe2 monolayer. We consider that these processes occur on the pristine 1H_MoSe2 monolayer and in the vicinity of an isolated Se vacancy. The presence of a single Se vacancy both enhances the molecular adsorption and reduces the energy needed for dissociation, making it energetically favorable for the case of O2 and NO molecules. Moreover, the presence of a second Se vacancy makes the dissociation process energetically favorable for all the molecules that are studied here. For each case we evaluate the effect that each adsorbate has on the electronic structure of the MoSe2 monolayer and the charge transfer that takes place between the adsorbate and the surface. Remarkably, adsorption of either CO or NO at the Se vacancy induces a finite spin-magnetization in the system that is spatially well localized around the adsorbate and the three closest Mo atoms.

Sara Conti

University of Antwerp

Chester supersolid of spatially indirect excitons in double-layer semiconductor heterostructures

A supersolid, a counter-intuitive quantum state in which a rigid lattice of particles flows without resistance, has to date not been unambiguously realised. Here we reveal a supersolid ground state of excitons in a double-layer semiconductor heterostructure over a wide range of layer separations outside the focus of recent experiments. This supersolid conforms to the original Chester supersolid with one exciton per supersolid site, as distinct from the alternative version reported in cold-atom systems of a periodic modulation of the superfluid density. We provide the phase diagram augmented by the supersolid. This new phase appears at layer separations much smaller than the predicted exciton normal solid, and it persists up to a solid–solid transition where the quantum phase coherence collapses. The ranges of layer separations and exciton densities in our phase diagram are well within reach of the current experimental capabilities.

Nguyen Duy Hoang Minh

Donostia International Physics Center

Synthetic Weyl semimetal and quantum anomalous Hall state in one-dimensional system of trilayer photonic grating

We study the spectral properties of a one-dimensional (1D) trilayer photonic grating in a 3D hybrid momentum space with the interlayer shifts playing the role of two synthetic momenta besides the genuine one of our 1D system. As the synthetic momenta are even under the time-reversal operation, this family of 1D lattice can host states that are often realized in systems with time-reversal symmetry broken. We find that highly tunable Weyl semimetal, nodal line semimetal, and quantum anomalous Hall state can be realized in our trilayer system. The results show that multilayer photonic grating is not only a promising platform for studying higher-dimensional topological physics but also a simple one for mimicking systems with broken time-reversal symmetry.

Juan Pablo Echeverry

Universidad de Ibagué, Ibagué-Colombia

Is Frozen Plasmon an Observable Signature of Exciton Condensation in 1T-TiSe2?

Searching the exciton insulator (EI), a Bose-Einstein condensation state of excitons, is of fundamental significance, but lacks determinant experimental evidences so far. A plasmon with energy freezing to zero at a finite momentum, which requires a breakdown of the Landau damping, has been proposed to be a signature of the EI in a condensed matter system. Here, using a surmised EI candidate 1T-TiSe2 as an example, we employ_first-principles calculations to study the plasmon damping. We demonstrate that the plasmon in TiSe2 does not survive in large momentum range due to the unavoidable Landau damping, so that the frozen plasmon cannot exist. The verification of EI needs further experimental evidences.

Paulo Eduardo de Faria Junior

University of Regensburg

First-principles insights into the spin-valley physics of strained transition metal dichalcogenides monolayers

Transition metal dichalcogenides (TMDCs) are ideal candidates to explore the manifestation of spin-valley physics under external stimuli. In this study, we investigate the influence of strain on the spin and orbital angular momenta, effective g-factors, and Berry curvatures of several monolayer TMDCs (Mo and W based) using a full ab initio approach. At the K-valleys, we find a surprising decrease of the conduction band spin expectation value for compressive strain, consequently increasing the dipole strength of the dark exciton by more than one order of magnitude (for 1-2% strain variation). We also predict the behavior of direct excitons g-factors under strain: tensile (compressive) strain increases (decreases) the absolute value of g-factors. Strain variations of 1% modify the bright (A and B) excitons g-factors by 0.3 (0.2) for W (Mo) based compounds and the dark exciton g-factors by 0.5 (0.3) for W (Mo) compounds. Our predictions could be directly visualized in magneto-optical experiments in strained samples at low temperature. Additionally, our calculations strongly suggest that strain effects are one of the possible causes of g-factor fluctuations observed experimentally. By comparing the different TMDC compounds, we reveal the role of spin-orbit coupling (SOC): the stronger the SOC, the more sensitive are the spin-valley features under applied strain. Consequently, monolayer WSe2 is a formidable candidate to explore the role of strain on the spin-valley physics.
We complete our analysis by considering the side valleys, _ and Q points, and by investigating the influence of strain in the Berry curvature. In the broader context of valley- and strain-tronics, our study provides fundamental microscopic insights into the role of strain in the spin-valley physics of TMDCs, which are relevant to interpret experimental data in monolayer TMDCs as well as TMDC-based van der Waals heterostructures.

Manato Fujimoto

Department of Physics, Osaka University

Perfect one-dimensional interface states in a twisted stack of three-dimensional topological insulators

We theoretically study the electronic structure of interface states in a twisted stack of three-dimensional topological insulators (3DTIs). By using a continuum model, we demonstrate that the interface band structures are completely different depending on the position of the Dirac cone, hosted on the surface of 3DTI, in the Brillouin zone. When the center of the surface Dirac cone is located at the center of BZ, the surface states are found to be simply gapped out when arranged in a twisted interface. When the center of the surface Dirac cone is at a midpoint of a side of BZ boundary, on the other hand, we find that the surface Dirac cones of top and bottom surfaces are converted to a perfect 1D channel, which is completely flat in one direction while disperses in the other direction. There, the left-going and right-going modes hosting opposite spin textures generates a spin current with opposite spin for upper and lower 3DTI's surface. they are robust against scattering by spin-independent impurities. Moreover, these peculiar 1D bands can be analytically understood as Landau levels of a formally equivalent lattice model, where the twist angle works as a fictitious magnetic field.

Augusto Ghiotto

Columbia University

Quantum criticality in twisted transition metal dichalcogenides

Near the boundary between ordered and disordered quantum phases, several experiments have demonstrated metallic behaviour that defies the Landau Fermi paradigm. In moiré heterostructures, gate-tuneable insulating phases driven by electronic correlations have been recently discovered. Here, we use transport measurements to characterize metal–insulator transitions (MITs) in twisted WSe2 near half filling of the first moiré subband. We find that the MIT as a function of both density and displacement field is continuous. At the metal–insulator boundary, the resistivity displays strange metal behaviour at low temperatures, with dissipation comparable to that at the Planckian limit. Further into the metallic phase, Fermi liquid behaviour is recovered at low temperature, and this evolves into a quantum critical fan at intermediate temperatures, before eventually reaching an anomalous saturated regime near room temperature. An analysis of the residual resistivity indicates the presence of strong quantum fluctuations in the insulating phase. These results establish twisted WSe2 as a new platform to study doping and bandwidth-controlled metal–insulator quantum phase transitions on the triangular lattice.

Raúl Ignacio Guerrero Avilés

Donostia International Physics Center

Topological/defect interplay using line array patterned on bilayer graphene

Gating Bernal bilayer graphene breaks inversion symmetry so that within the gap, stacking AB/BA boundaries show topological protected gapless states. Here, we consider electron-electron interactions within density functional theory to study arrays where the AB and BA domains are patterned periodically using pentagons-octagons defect-lines. We find that a gap is opened because of patterning where the topological states are still seen. In addition the defect lines introduce spin-polarized states pinned near the Fermi level, which are being ferromagnetically coupled under small magnetic fields. In fact, magnetic and topological states are mixing and show conducting channels with spin-momentum locking, an effect that partially persists even with n-doping and gate voltage. Furthermore, along the lines and under n-doping, the defect bands can be nested at the Fermi surface causing modulated charge densities that are nearly commensurated with the underlying graphene lattice. One dimensional arrays have then shown a new kind of transport channels than could be interesting further in the area of valleytronics.

Masaru Hitomi

Department of Physics, Osaka university

Quasi-band approach for the twisted bilayer quasicrystals

We propose a general theoretical approach to calculate the response function in non-periodic twisted bilayer systems. It is well known that a twist bilayer with low twist angle can be approximately treated as a periodic Bloch system with a moire superlattice period. When arbitrary 2D materials are overlaid with an arbitrary rotation angle, however, there are generally no noticeable effective periods and the system becomes truly quasiperiodic. A typical example of this is a 30-degree twisted bilayer graphene [1], where the electronic structure exhibits a quasi-periodic pattern with 12-fold rotational symmetry. It is generally difficult to calculate the physical quantities in such systems because the Bloch theory is not applicable.

In this work, we propose a theoretical framework to define the quasi band and calculate response function for general twisted bilayer quasicrystals. We first construct the Hamiltonian in k-space bases with a certain cut-off and calculate the quasi-band structure. The velocity operator can be computed by differentiating the Hamiltonian in k-space, and the optical absorption spectrum (dynamic conductivity) is obtained just as in the usual Bloch system. Here we demonstrate this prescription for the 1D and 2D twisted bilayer systems.

[1] P. Moon, M. Koshino, Y-W. Son, Phys. Rev. B 99. 165430 (2019).

Rebecca Hoffmann

ICFO - The Institute of Photonic Sciences

Electrostatic spatial control of graphene plasmon polaritons

Graphene plasmons possess large momenta over a very large bandwidth and hence confine light on the nanoscale. To spatially control graphene plasmons, one can exploit plasmon reflection, for example by engineering two regions where the plasmons momentum is notably different. However, despite extensive efforts it has not been demonstrated, primarily because the reflection coefficient strongly depends on the sharpness of the electrostatically induced potential, which was the limiting factor so far.

Here, we present a new lithography-free high-resolution fabrication technique that is capable of patterning sharp single feature as well as periodic structures with a world-record resolution, on the sub-20nm scale. Using this method, we build plasmonic graphene devices, where sharp potential features are electrostatically induced in the graphene layer. We then use scattering-type scanning near-field optical microscopy to investigate the graphene plasmon reflection induced by the sharp electrostatic profile generated with the patterned gate. Our experiments conclusively demonstrate electrostatically induced plasmonic reflection, paving the way to a range of new designs and devices, including electrostatically induced plasmonic cavities, waveguides and plasmonic metamaterials.

Zhihao Jiang

Aarhus University

Mapping angle- and doping-dependent dispersion of bending graphene

The possibility to systematically engineer the interlayer rotation angle θ between two-dimensional (2D) materials stacked in heterostructures offers an intriguing means to tailor superlattices, electronic band structures and interactions. Here, we set out to perform a proof-of-principle nanoARPES experiment demonstrating the ability to continously twist a graphene flake stacked on hexagonal boron nitride by tuning θ using a nano-rotation device engaged by the tip of an atomic force microscope (AFM). The overarching objective is thereby to capture the evolution of the θ-dependent electronic dispersion of graphene. Ultimately, these experiments are expected to pave the way for band structure measurements of systematically twisted heterostructures composed of bilayer graphene and monolayer dichalcogenides.

Alejandro Jimeno-Pozo

IMDEA Nanoscience

Superconductivity from repulsive interactions in Bernal Bilayer Graphene

The emergence of superconductivity in Bernal Bilayer Graphene (BBG) is discussed through a Kohn-Luttinger-like approach. This mechanism simply considers the screening of the purely long-range Coulomb potential between states in the same valley as responsible of the effective interaction that give rise to the superconducting phase in the continuum model of BBG. We find a critical temperature of the order of tens of mK which agrees approximately with the experimental observations. The inclusion of a Hubbard- like inter-valley interaction shows that the order parameter changes sign between valleys, thus indicating that BBG is a spin-triplet superconductor. We also check out the validity of this mechanism in the case of Rhombohedral Trilayer Graphene (RTG).

Alfred Jones

Aarhus University

Viewing engineered massive Dirac quasiparticles in lithographic superstructures

Massive Dirac quasiparticles play a central role in a number of emerging physical phenomena such as topological phase transitions and anomalous Hall effects. Single-layer graphene appears to be an ideal platform to explore such properties, however engineering the transition from massless to massive Dirac quasiparticles in a controllable fashion remains a significant challenge. Here, we employ angle-resolved photoemission with a nanoscale light spot (nanoARPES) to directly measure the electronic structure modifications induced by lithographic patterning of an antidot superlattice onto a graphene device. We observe a transition from massless Dirac fermions in the pristine graphene to a massive character in patterned regions, and determine that the mass scales linearly with antidot diameter, consistent with theory. Gate-induced electron-doping of the patterned graphene produces an enhancement of the mass, highlighting the versatility of nanopatterned graphene as a platform for engineering such quasiparticles.

Ekaterina Khestanova

ICFO

Robustness of momentum-indirect interlayer excitons in MoS2/WSe2 heterostructure against charge carrier doping

Monolayer transition-metal dichalcogenide (TMD) semiconductors exhibit strong excitonic effects and hold promise for optical and optoelectronic applications. Yet, electron doping of TMDs leads to the conversion of neutral excitons into negative trions, which recombine non-radiatively at room temperature. As a result, the photoluminescence (PL) intensity is quenched. Here we study the optical and electronic properties of a MoS2/WSe2 heterostructure as a function of chemical doping by Cs atoms performed under ultra-high vacuum conditions. By PL measurements we identify two interlayer excitons and assign them to the momentum-indirect Q-_ and K-_ transitions. The energies of these excitons are in a very good agreement with ab initio calculations. We find that the Q-_ interlayer exciton is robust to the electron doping and is present at room temperature even at a high charge carrier concentration (10^13 cm_2). Submicrometer angle-resolved photoemission spectroscopy (ARPES) reveals charge transfer from deposited Cs adatoms to both the upper MoS2 and the lower WSe2 monolayer without changing the band alignment. This leads to a small (10 meV) energy shift of interlayer excitons. The robustness of the momentum-indirect interlayer exciton to charge doping opens up an opportunity of using TMD heterostructures in devices requiring both light emission and a high carrier density.

Xueheng Kuang

IMDEA Nanoscience and Wuhan University

Flat-band plasmons in twisted bilayer transition metal dichalcogenides

Twisted bilayer transition metal dichalcogenides are ideal platforms to study flat-band phenom_ena. In this paper, we investigate flat-band plasmons in hole-doped twisted bilayer MoS2 by em_ploying a full tight-binding model and the random phase approximation. We find that, in samples with lattice relaxations, the flat band is not separated from other valence bands by a forbidden energy gap, which makes the contribution of interband transitions have a significant difference in transforming plasmon dispersion and energy. In particular, low-damped and quasi-flat plasmons emerge if we only consider intraband transitions in the doped flat band, whereas a two-dimensional classical plasmon dispersion emerges if we also take into account interband transitions between the flat band and remote bands. Furthermore, the plasmon energies are tunable also with twist angle and doping level. Strongly enhanced interband transitions at a higher dop_ing level will quench the quasi-flat plasmons. However, in a rigid sample, lower-energy quasi-flat plasmons and higher-energy interband plasmons can coexist. Based on the relaxation effect and doping effects, we conclude that the two conditions, isolated flat band and properly hole-doping level, are essential for observing the low-damped and quasi-flat plasmon mode in twisted bilayer transi_tion metal dichalcogenides. We hope that our study on flat-band plasmons can be instructive for studying the possibility of plasmon-mediated superconductivity in twisted bilayer transition metal dichalcogenides in the future.

Kai-Qiang Lin

University of Regensburg

Excitonic quantum interference in 2D semiconductors

Few solid-state systems exhibit optical phenomena related to quantum interference such as electromagnetically induced transparency (EIT). We demonstrate a cavity-free, atom-like EIT effect in an excitonic three-level system formed in single-layer crystals of WSe2 [1,2]. We probe EIT by second-harmonic generation (SHG), which is possible because of broken inversion symmetry. Under the condition of double resonance of the driving and radiated field with the fundamental excitonic transitions, the SHG spectrum splits due to excitonic quantum interference. The number of dips in the SHG spectrum relates directly to the number of Rabi flops the strongly driven system undergoes within a single laser pulse. The coherent dynamics are accurately described by a ladder-type three-level model. We further demonstrate the ability to control EIT through twist angle in bilayer WSe2 and MoSe2 [3]. Such a degree of freedom does not exist in conventional dilute atomic-gas systems, where EIT was originally established, and allows us to shape the frequency dependence, i.e., the dispersion, of the optical nonlinearity.

[1] K.-Q. Lin et al., Nat. Phys. 15, 242-246 (2019).
[2] K.-Q. Lin et al., Nat. Commun. 12, 5500 (2021).
[3] K.-Q. Lin et al., Nat. Commun. 12, 1553 (2021).

Yulia Maximenko

NIST/UMD

Mapping narrow bands in electrostatically tunable twisted double bilayer graphene

Artificial superlattices in 2D materials proved to be versatile platforms for band engineering and studying correlated quantum phases. Due to the additional periodic potential, flat-band phase can be induced in a crystal leading to strong electron-electron interactions. Specifically in twisted moiré heterostructures, this periodicity is controlled by tuning the angular misalignment between layers. In magic angle twisted bilayer graphene, flat bands and correlated quantum phases appear only at a few precise values of the twist angle. In contrast, small-angle twisted double bilayer graphene (TDBG) can be electrostatically tuned into the correlated regime for a range of twist angles. Local probe measurements are key to avoid the common complication of twist angle disorder in global transport studies. Here we employ scanning tunneling and atomic force microscopy together with electrostatic gating to study TDBG with atomic spatial and high energy resolution in magnetic fields up to 15 T. We observe magnetic-field-induced quantization and use it to explore the dramatic band structure changes in response to electric field. We use theoretical modeling of the effects of displacement fields, Berry curvature, and magnetic fields to support our experimental findings.

Johannes Motruk

University of Geneva

Kagome and spin liquid physics in transition metal dichalcogenide bilayers

Bilayers of transition metal dichalcogenides (TMDs) have recently emerged as promising platforms to study strongly correlated electrons in two dimensions. In particular, the low-energy physics of these systems can be described by generalized Hubbard models on the triangular lattice. At certain fillings and parameter regimes, generalized Wigner crystals can occur in which the translational invariance of the charge distribution is spontaneously broken. In this work, we investigate TMD heterobilayers at a filling of 3/4 holes or electrons per moiré unit cell where these are almost entirely localized on a kagome lattice. By expanding the tight-binding model describing the system, we derive an effective spin model on this kagome lattice that includes up to third-neighbor Heisenberg and Dzyaloshinskii–Moriya interactions. Through a combination of density matrix renormalization group simulations and Schwinger boson mean field analysis, we explore the possibilities of realizing quantum spin liquids in this model in experimentally realistic parameter ranges and show that a chiral spin liquid is a competitive ground state candidate.

Daniel Muñoz-Segovia

Donostia International Physics Center (DIPC)

Superconducting collective Leggett modes in single-layer 1H-NbSe2

While bulk 2H-NbSe2 is generally accepted to be a conventional superconductor, several unconventional features of the superconducting state have been reported in the monolayer limit, including the breaking of threefold symmetry in magnetotransport [1,2] and anomalously large in-plane critical fields [3]. In this work, I will first present another unconventional feature measured by our collaborators [4]: the existence of satellite peaks in the STM spectra of 1H-NbSe2 monolayers which exist only in the superconducting state and show a clear anticorrelation with the superconducting gap. After briefly discussing other potential candidate explanations, I will propose a scenario of competing pairing between s-wave and subleading f-wave triplet channels that leads to a superconducting Leggett collective mode. In particular, I will present a calculation of the Leggett mode energy using a simplified continuum model for NbSe2, and show that this particle-particle collective mode gives rise to resonances in the tunneling spectrum. I will discuss how our model compares with the experimental data, discuss the origin of the anticorrelation, and argue that it provides support to the competing pairing scenario, with a sizable attraction in the subleading triplet channel.

[1] A. Hamill, et al., Nat. Phys. 17, 949–954 (2021).
[2] C.-W. Cho, et al., arXiv:2003.12467 (2020).
[3] M. Kuzmanovi_, et al., arXiv:2104.00328 (2021).
[4] W. Wan, et al., arXiv:2101.04050 (2021).

Iris Niehues

CIC Nanogune

Nanoscale mapping of carrier density in intercalated 2D semiconductors by IR and THz nanoscopy

Intercalation of 2D semiconductors, such as MoS2, with molecules is interesting because it drastically changes the electric, optical, and magnetic properties of the host crystal. In order to observe and understand the intercalation process and its impacts on the material properties, it is crucial to gain knowledge about the molecule distribution in the semiconductor. Here we use near field techniques to show that Tetraethylammonium (TEA) molecule intercalation of MoS2 bulk crystals locally changes the conductivity. The techniques are based on elastic light scattering at an atomic force microscope tip, employing monochromatic laser illumination or broadband illumination from an IR supercontinuum laser. Acting as an optical antenna, the tip converts the illuminating field into a strongly concentrated near field at the very tip apex (nanofocus). Recording of the tip-scattered field as a function of sample position (monochromatic illumination) yield nanoscale-resolved IR/THz images (s-SNOM), while Fourier-transform spectroscopy of the tip-scattered field (broadband illumination) allows for nanoscale IR point spectroscopy (nano-FTIR). In the s-SNOM images we find a drop of the amplitude signals with increasing frequency, and a change of the phase contrast, resembling a Drude-like response, while the pristine MoS2 shows no changes with frequency. Furthermore, the amplitude and phase images of the intercalated MoS2 flakes are not homogeneous, indicating a spatial variation of the local conductivity, i.e., the carrier concentration. In addition, we use nano-FTIR to measure the molecular vibrations showing the presence and amount of the TEA molecules. Generally, our work shows the potential of IR/THz nanoimaging as a noninvasive technique to simultaneously map the carrier concentration together with molecular vibrations, thus allowing for correlating the presence of molecules with the conductivity of the system.

Claudia Maria Pereira Cardoso

Center S3, CNR Institute of Nanoscience, Modena, Italy

Electrically tunable hybridization magnetic proximity effect

Conventional magnetic proximity effect is portrayed as a spin splitting induced in the energy levels of a non-magnetic material because of its exchange interaction with an underlying magnetic material, that lead to spin-dependent properties in the non-magnetic material. This effect is usually small, on account of the small proximity induced splitting. Here we propose a new class of magnetic proximity effect based on the spin dependent hybridization of the electronic states at the Fermi energy of a non-magnetic conductor with narrow spin split bands of a ferromagnetic insulator and we show it can be very large and electrically tunable. We illustrate this effect in the case of Dirac electrons in monolayer graphene with the spin-polarized flat conduction band of a CrI3 and we show the proposed effect opens up gap in one spin channel only, making graphene half-metallic. We show that an off-plane electric field controls the hybridization and we propose very efficient spin valve based on hybridization proximity.

Jose Manuel Pereira Sanchez

CIC nanoGUNE BRTA

Superconductivity in organic-ion intercalated MoS2

Upon reaching a particular charge carrier density, MoS2 can develop a charge density wave and turn superconductive REF1, making it a promising material for quantum computation. However, the required doping levels are typically achieved using ionic-liquid gating or air-sensitive alkali-ion intercalation REF2, which are not compatible with standard device fabrication processes. Here, we report on the emergence of superconductivity and of a charge density wave in MoS2 intercalated with air-stable organic cations. By selecting two different molecular guests, we show that these correlated electronic phases depend dramatically on the intercalated cation, demonstrating the potential of organic ion intercalation to finely tune the properties of 2D materials. Moreover, we find that a fully developed zero-resistance state is not reached in few-nm-thick flakes, indicating the presence of three-dimensional superconductive paths which are severed by the mechanical exfoliation.

REF1: Ye, J. T., Yj J. Zhang, R. Akashi, Ms S. Bahramy, R. Arita, and Y. Iwasa. ""Superconducting dome in a gate-tuned band insulator."" Science 338, no. 6111 (2012): 1193-1196.

REF2: Zhang, Renyan, I-Ling Tsai, James Chapman, Ekaterina Khestanova, John Waters, and Irina V. Grigorieva. ""Superconductivity in potassium-doped metallic polymorphs of MoS2."" Nano letters 16, no. 1 (2016): 629-636."

Giuseppe Ronco

University of Rome - La Sapienza

Redistribution and g-Factor Tuning of Localized Excitons in Site-controlled Quantum Emitters by Reversible Strain Fields

Localized excitons in monolayer transition metal dichalcogenides (ML-TMDs) are attracting considerable interest for their capability to generate single photons with high brightness [1]. Since both spatial strain gradients[2] and defects play a crucial role in inducing single photon emission, achieving dynamic control of strain fields in 2D materials can thus allow us to engineer the quantum emitters' properties and to exploit their full potential for quan-tum technologies.

In this work, we show how strain fields provided by ordered arrays of piezoelectric micro-pillars can be used to both control the nucleation site of quantum emitters and dinamically modify their emission properties [3,4]. In particular, we demonstrate that the energy of lo-calized excitons in ML WSe_2 can be precisely tuned across a spectral range as large as tens of meV with no change in the multi-photon emission probability [3]. We observed that the applied strain modifies in a reversible way the emitters' distribution, thus allowing for a con-trollable tuning of their optical properties. We also provide a theoretical model based on the diffusion equations for the exciton in presence of strain fields that explains the experimental results we found[4]. Furthermore, we exploited deformation fields to fine tune the g-factor of the emitters, allowing for the investigation of their response in presence of magnetic field.

Since ML-TMDs offer unique optical and electronical properties such as inversion sym-metry breaking, strong light-matter interaction, large spin-orbit coupling and valley selective optical selection rules, efficient TMDs-based single photon sources could open to novel possibilities in advanced quantum optics protocols. Our hybrid ML-TMDs-piezoelectric platform bursts into this context, providing a simple method to fabricate ordered arrays of single photon sources with tuneable energy.

[1] A. Srivastava, et al., Nature Nanotechnology 10, 491, (2015).
[2] M. Koperski, et al, Nature Nanotechnology, 10, 497, (2015).
[3] O. Iff, et al, Nano Lett, 10, 6931, (2019).
[4] M. Savaresi et al., in preparation (2022).

Héctor Sainz Cruz

IMDEA Nanociencia

Current-phase relation in twisted bilayer graphene Josephson junctions

Twisted multilayers of graphene enable the creation of monolithic superconducting devices. Here, we calculate the current-phase relation in twisted bilayer graphene Josephson junctions, doing exact diagonalization on a Bogoliubov-de Gennes, scaled tight-binding Hamiltonian which includes the Hartree correction. The current-phase relation shows significant skewness and changes non-monotonically with twist angle, reaching its maximum value away from the magic angle of 1.06º. We compare s-wave pairing with a topological pairing that breaks time reversal symmetry and discuss signatures of hybrid topological/non-topological junctions.

Mathias Scheurer

University of Innsbruck

Zero-field superconducting diode effect in twisted trilayer graphene

The semiconducting diode, which is characterized by a highly asymmetric current-voltage relation, is central to modern-day electronics. In the last few years, its superconducting analogue – a system that behaves like a superconductor for current flow in one direction but exhibits finite resistance when the current direction is reversed – has attracted attention in the physics community, due to its potential for future quantum-electronics applications. So far, this behavior has only been realized in the presence of a magnetic field, magnetic junction or magnetic proximity. On this poster, I will discuss experimental evidence and a microscopic theory for a strong superconducting diode effect at zero external magnetic in twisted trilayer graphene [1-3]. I will discuss why this is a natural system to realize this exotic superconducting behavior as an intrinsic property and illustrate the intricate underlying microscopic physics.

[1] Siriviboon, Lin, Scammell, Liu, Rhodes, Watanabe, Taniguchi, Hone, MS, Li, arXiv:2112.09115.
[2] Lin, Siriviboon, Scammell, Liu, Rhodes, Watanabe, Taniguchi, Hone, MS, Li, and arXiv:2212.07841.
[3] Scammell, Li, MS, arXiv:2112.09115.

Jose Angel Silva Guillén
IMDEA Nanociencia

An atomistic study of the effect of substrates on the structural and electronic properties of Twisted Bilayer Graphene

Twisted bilayer graphene (TBG) has taken the spotlight of the scientific community for the past few years due to the finding of superconductivity at the so-called “magic angles” as well as other strong correlated states such as Mott insulating phases [1,2].
In experimental devices, TBG is usually deposited on top of a substrate such as hexagonal boron nitride (hBN). Although the effect of the substrate on the structural and electronic properties of TBG has been studied before, it has been done in a perturbative way, for example, using continuum models [3,4].
In this work [5], we have gone one step further and have studied heterostructures of TBG and hexagonal boron nitride (hBN) using an atomistic tight-binding (TB) model together with semi-classical molecular dynamics to consider relaxation effects. Since TBG can be either supported or clamped between hBN layers we have studied both cases.
We have found that hBN affects the electronic properties of TBG. In the case of TBG supported on hBN we have seen that hBN influences the electronic properties of TBG even for angles far from alignment. Furthermore, a gap that separates the flatbands appears in the system. We attribute this opening to a mass gap induced by the presence of the hBN substrate. Interestingly, these bands also split due to the combination of the mass gap and a pseudo-magnetic field induced by hBN. This splitting is also a consequence of the breaking of the layer degeneracy.
When TBG is clamped between two layers of hBN, we have found that the gap is still present in the system, although the layer degeneracy can be recovered for certain angles.
As we have said before, the use of continuum models to study these kinds of systems is very extended mainly due to the large number of atoms present in the supercell. Therefore, it is key that these models correctly describe the TB calculations. For this, we have developed a continuum model and we have found that the substrate-induced potential needs to be expanded up to two harmonics.
Therefore, our approach that combines molecular dynamics with TB calculations could be key for the explanation of the interesting phenomena found in TBG experiments.

[1] Y. Cao, et al. Nature 556, 43-50 (2018)
[2] Y. Cao, et al. Nature 556, 80-84 (2018)
[3] M. Koshino, et al. Phys. Rev. X. 8, 031087 (2018)
[4] F. Guinea and N. R. Walet. Phys. Rev. B 99, 205134 (2019).
[5] M. Long, et al. npj Computational Materials (In Press, 2022)

Andreas Sinner

IMDEA Nanosciencia

Pairing transition in a heterogeneous double layer with interlayer Coulomb repulsion

We study the interlayer pairing states in layered systems of two different 2d electronic subsystems, one with relativistic linear and the other with non-relativistic parabolic spectrum. The complex order parameter of the paired state has a two component structure. We investigate the pairing state formation on the mean-field level, determine the critical interaction strength and evaluate the effective potential. The anisotropic three-band spectrum of quasiparticles depends explicitly on the phase difference of the order parameter components, rotates in momentum space as it changes. It is subject to the strong band deformation due to the pairing. It leads to the fusion and hybridization of initially decoupled bands. The quasiparticle spectrum has the shape of deformed Dirac cones in the vicinity of the two touching points between neighboring bands. The density of states exhibits a number of specific features due to band deformation, such as a van Hove singularity.

Manuel Suárez-Rodríguez

CIC nanoGUNE BRTA

Gate-tuneable and chirality-dependent charge-to-spin conversion in tellurium nanowires

Chiral materials are an ideal playground for exploring the relation between symmetry, relativistic effects and electronic transport. For instance, chiral organic molecules have been intensively studied to electrically generate spin-polarized currents in the last decade, but their poor electronic conductivity limits their potential for applications. Conversely, chiral inorganic materials such as tellurium have excellent electrical conductivity, but their potential for enabling the electrical control of spin polarization in devices remains unclear. Here, we demonstrate the all-electrical generation, manipulation and detection of spin polarization in chiral single-crystalline tellurium nanowires. By recording a large (up to 7%) and chirality-dependent unidirectional magnetoresistance, we show that the orientation of the electrically generated spin polarization is determined by the nanowire handedness and uniquely follows the current direction, while its magnitude can be manipulated by an electrostatic gate. Our results pave the way for the development of magnet-free chirality-based spintronic devices.

Bilal Tanatar

Department of Physics, Bilkent University, Turkey

Metal-insulator transitions in electron-hole bilayer transition metal dichalcogenides

We investigated metal-insulator transitions for double-layer two-dimensional electron-hole systems in transition metal dichalcogenides stacked on opposite sides of thin layers of boron nitride. The interparticle interaction is calculated by including the screening due to the polarization charges at different interfaces, including that at the encapsulation and at the substrate of experimental structures. We compute and compare the energies of the metallic electron-hole plasma and the proposed insulating exciton solid with fixed-node diffusion Monte Carlo simulation including the high valley degeneracy of the electron bands. We found that for some examples of current experimental structures, the transition electron/hole density is in an experimentally accessible range between 4.1 10^{12} cm^{-2} and 14.5 10^{12} cm^{-2} for spacer thicknesses between 2.5 and 7.5 nm.

Tarun Tummuru

University of British Columbia

Topological superconductivity in twisted cuprates

Various phenomena occur when two-dimensional materials, such as graphene or transition metal dichalcogenides, are assembled into bilayers with a twist between the individual layers. As an application of this paradigm, we predict that structures composed of two monolayer-thin d-wave superconductors with a twist angle can form a gapped topological phase with spontaneously broken time-reversal symmetry and protected chiral Majorana edge modes. These structures can be realized by mechanically exfoliating van der Waals-bonded high-Tc cuprates, such as BSCCO. Symmetry arguments and microscopic modelling suggest that this phase will form for a range of twist angles in the vicinity of 45deg, and will set in at a temperature close to the bulk superconducting critical temperature of 90K. This platform may, therefore, provide a realization of a high-temperature topological superconductor.

Marc Vila Tusell

University of California, Berkeley and Lawrence Berkeley National Lab

Valley-polarized quantum anomalous Hall phase in bilayer graphene with layer-dependent proximity effects

Realizations of some topological phases in two-dimensional systems rely on the challenge of jointly incorporating spin-orbit and magnetic exchange interactions. Here, we predict the formation and control of a fully valley-polarized quantum anomalous Hall effect in bilayer graphene, by separately imprinting spin-orbit and magnetic proximity effects in different layers. This mechanism contrasts with other proposals of this effect where both interactions are needed in both layers and as such poses challenges for experimental realizations. Our model results in varying spin splittings for the conduction and valence bands, which gives rise to a topological gap at a single Dirac cone. The topological phase can be controlled by a gate voltage and switched between valleys by reversing the sign of the exchange interaction. By calculating the valley-resolved Hall conductivity together with quantum transport simulations in disordered systems, the chirality and resilience of the valley-polarized edge states are demonstrated. Our findings provide a promising route to engineer a topological phase that could enable low-power electronic devices and valleytronic applications as well as putting forward layer-dependent proximity effects as a way to create versatile topological states of matter.

Daniel Wigger

School of Physics, Trinity College Dublin, Ireland

A new destructive photon echo in six-wave mixing signals from local field coupling in a MoSe2 monolayer

Two-dimensional semiconductors, especially in the form of transition metal dichalcogenides, are a widely investigated subject in several areas of physics for the last couple of years. One of the reasons for this is their strong excitonic optical response. This allows to efficiently perform ultrafast nonlinear spectroscopy on these systems to learn about their fundamental physical processes.

We have recently studied how the spectral dynamics of pump-probe [1] and four-wave mixing signals [2] can be explained by an exactly solvable model that extends the basic Bloch equations by a local field effect. This local field coupling takes into account the interaction between the optically generated excitons in the 2D systems on a mean field level and leads to spectral shifts depending on the excitonic occupation.

We then went a step further and studied six-wave mixing signal dynamics and discovered a peculiar temporary signal depression, depending on the considered delay between the two applied laser pulses [3]. In this contribution, we will report on this experimental finding and demonstrate that the observed signal dynamics can be understood as a new destructive photon echo effect. With our local field model we are able to attribute this feature to the interaction between the excitons. Inspired by the Bloch vector interpretation of the original photon or spin echo effect, we also developed an illustration on this level for the destructive echo, and show that the Bloch vectors contributing to the six-wave mixing signal form Lissajous figures.

[1] A. Rodek et al., Nanophotonics 10, 2717 -- 2728 (2021).
[2] T. Hahn et al., New J. Phys. 23, 023036 (2021).
[3] T. Hahn et al., Adv. Sci. 9, 2103813 (2022)."

Kevin Zhang

Cornell University

Fractons and solitons in moire systems

As a unique opportunity hosted by the magic angle twisted bilayer graphene (MATBG), the emergence of a novel fractional correlated insulating (FCI) state dictated by the geometry of the three-peak structure of Wannier orbitals has been proposed [1]. While Ref.[1] established the novel FCI state with extensive ground-state landscape at the filling of n±1/3 from rigorous considerations in the strong coupling limit, little is known about the nature of excitations. At the same time, novel correlated ground states often host unusual excitations. In this talk, I will discuss the nature of two distinct fractionalized excitations in the FCI phase. : (1) fracton-like vortices and (2) soliton-like domain wall edge states. Although both types of excitations carry fractional electric charges, their topological charges are distinct. Moreover, both defects' movements are restricted to emergent low-dimensional subspace embedded in the two-dimensional (2D) space of MATBG and hence ``fractonic''. Specifically, fractonic vortices are immobile while the domain wall edge states' motion is restricted along one direction, behaving much like a 2D version of solitons in a Su-Schriffer-Heeger chain. We discuss implications of these fractonic excitations on the band-width tuned and doping tuned phase transition from the fractional correlated insulator phase to the Fermi liquid phase. We also discuss how magnetism can intertwine with dynamics of the fractons. We propose experiments to pursue these fractons in the partially filled (n\pm1/3) magic angle twisted bilayer graphene is tantalizing.