Summer School

Simulation of van der Waals [hetero]structures

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Book of Abstracts

Yu-Shiba-Rusinov States in Ising superconductors

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Abstract

Recently there has been a huge effort to investigate individual magnetic impurities on superconducting surfaces in the context of scanning tunneling microscopy (STM) [1]. These STM-based experiments have enabled to elucidate the properties of the in-gap superconducting bound states known as Yu-Shiba-Rusinov states. These bound states are a key signature of the interplay between magnetism and superconductivity at the atomic scale and, in turn, lead to a strong local modification of the superconducting state. In this regard, we present our theoretical efforts to understand the physics of YSR states in Ising superconductors, which accommodate a spin-orbit field pinning the spins to the out of plane direction. We show that the study of YSR states can provide a very valuable way to reveal the underlying properties of unconventional superconductors.

Figures

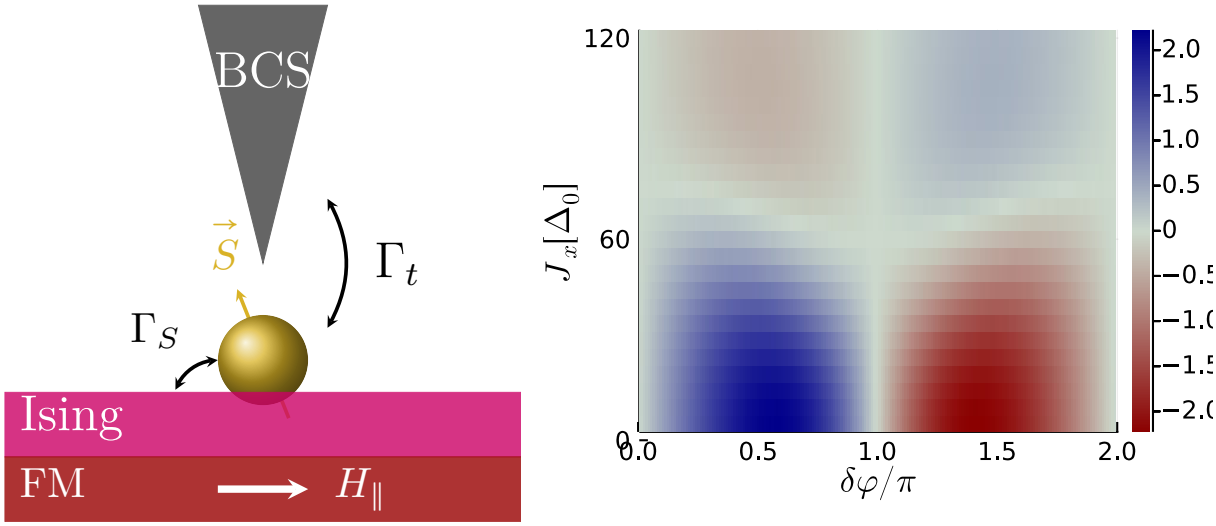

Figure 1: (left) Schematics of the setup under consideration: YSR states form due to strong coupling between the Ising superconductor and a magnetic impurity (by Γ_S). Further coupling to a BCS STM tip (by Γ_t) results in a Josephson current depending on strength and direction of the magnetisation of the impurity. (right) Josephson current phase relation for an impurity spin along the x-direction under the action of an in plane magnetic texture $H_\parallel$ on the superconductor.

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Electromagnetic Radiation Scattering of Free Monolayer Dielectric Microspheres with Different Size Parameters

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Abstract

Light scattering from dielectric microspheres has attracted considerable attention because of their unique characteristics, attributes, and great potential [1-4]. Herein, the results of numerical simulations of the near-field electromagnetic wave (EMW) distribution arising from dielectric microspheres are presented. While previous research focused on the EMW distribution intensity [4]; here, phase and vectorial representations alongside the intensity of the electric field are reported. This investigation aims to provide a comprehensive understanding of light behavior when interacting with dielectric microspheres in order to be used effectively as probes for spectroscopic investigation of few-atoms-thick 2D films [5].

Figures

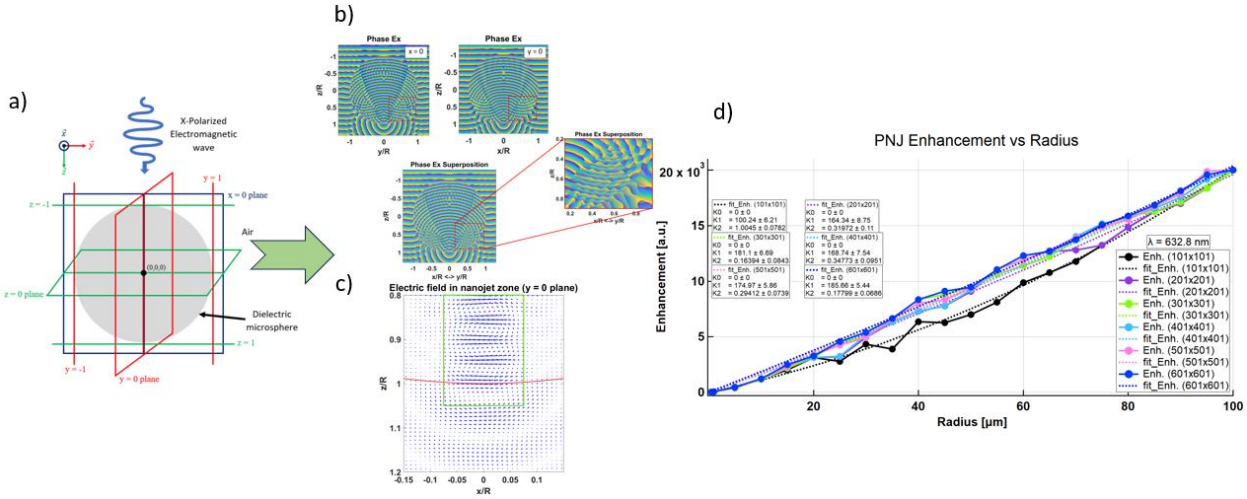

Figure 1: a) schematic illustration of incident light on free microsphere, b) phase plots of electric field's x, y components and their superposition, c) vectorial representation of photonic nanojet, d) Photonic nanojet maximum enhancement vs microsphere's radius.

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In silico tuning the properties of inorganic-organic hybrid systems

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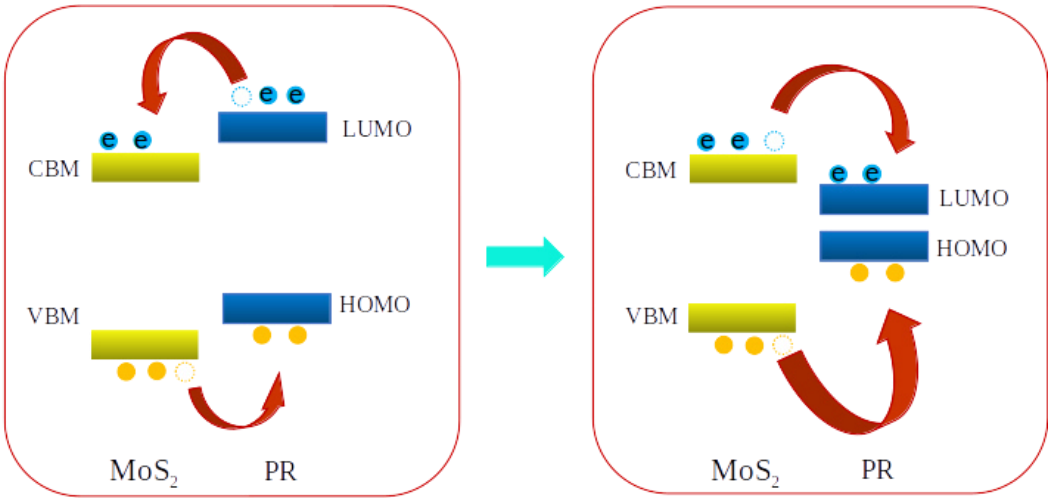
Abstract

Two-dimensional (2D) materials are expanding the range of processes that can be studied in two dimensions as well as in van der Waals (vdW) heterostructures. Integrating organic molecules into these systems has enormous potential because nature offers a finite number of 2D materials [1]. Still, an almost unlimited range of molecules can be tailored and synthesized with predictable properties. Organic compounds are widely known for their high absorption with low mobility and charge stability, whereas inorganic compounds have comparatively low absorption with excellent charge transport properties [2]. Thus, the formation of vdW heterostructures that combine an inorganic compound with organic molecules potentially offers the advantages of both. Molybdenum disulfide (MoS_2), one of the transition-metal dichalcogenides (TMDs), is one of the most exciting 2D semiconductors holding promises for potential applications in transistors, optoelectronics, and catalysis [1, 2]. Perylenes are widely used dyes whose optical properties can be tuned by chemical modification of the perylene core. Here we report on a systematic study of the structural, electronic, and optical properties of MoS_2/perylene hybrid systems by means of density functional theory. Using different perylenes (perylene orange, perylene diimide, and perylene red) highlights the extent to which property tuning can be achieved in the hybrid system.

Figures



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Dielectric Resonators for Increased Light-Matter Interaction

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Abstract

Harnessing optimal light-matter interactions is of paramount importance in the evolving landscape of photonics and optoelectronics. Dielectric resonators, characterized by low absorption losses and the ability to support Mie-type resonances, have emerged as pivotal tools in this endeavor. I present an exploration of dielectric resonators, from localized isolated structures to extended bound-state-in-the-continuum (BIC) ones, focusing on their capability to confine, control, and amplify electromagnetic fields [1]. I highlight the symbiotic relationship between dielectric resonators and active emitters, particularly quantum dots [2,3] and Transition Metal Dichalcogenides (TMD) materials, elucidating their combined potential in enhanced light emission and detection. Furthermore, I delve into the integration techniques of dielectric resonators with modern photonic devices. I amplify the real-world ramifications by emphasizing applications ranging from augmented reality, nonlinear optics, and even quantum computing. Conclusively, I suggest that dielectric resonators, when synergized with active emitters and tailored through advanced designs, are poised to redefine the horizons of nanophotonics and optoelectronics.

Figures

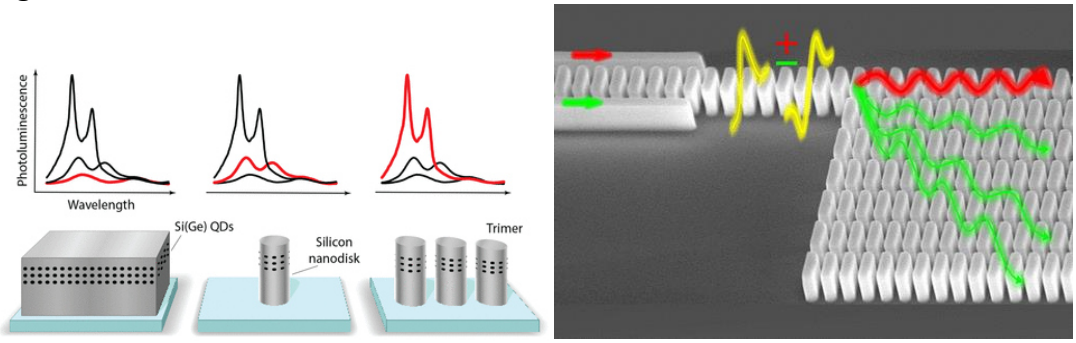

Figure 1: Luminescence enhancement and coherent light control in coupled resonators

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3D Electron Diffraction on Nano-Lamellae of $Cu(Sb_2S_3)Cl$

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Abstract
The dark red semiconductor $Cu(Sb_2S_3)Cl$ was obtained by leaching the layered precursor $Cu(Sb_2S_3)[AlCl_4]$ in 0.1 M HCl.[1] Poor crystallinity of the product and misalignment of lamellae down to the nanoscale prevent structure determination by conventional single-crystal X-ray diffraction. The combination of transmission electron microscopy, selected area electron diffraction, and manual selected area electron precession diffraction tomography on a spot with largely ordered crystalline lamellae facilitated the ab initio determination of the crystal structures of two intergrown modifications. Orthorhombic o-$Cu(Sb_2S_3)Cl$ and monoclinic m-$Cu(Sb_2S_3)Cl$ have similar layers as the precursor consisting of uncharged Sb_2S_3 strands whose sulfide ions, together with chloride ions, coordinate the copper(I) cations. Only one chloride ion remained from the $[AlCl_4]^-$ group, while $AlCl_3$ was removed from the space between the layers. DFT calculations confirm the structure solution for the orthorhombic form and reveal that the monoclinic structure is metastable against a transformation to o-$Cu(Sb_2S_3)Cl$.

Figures

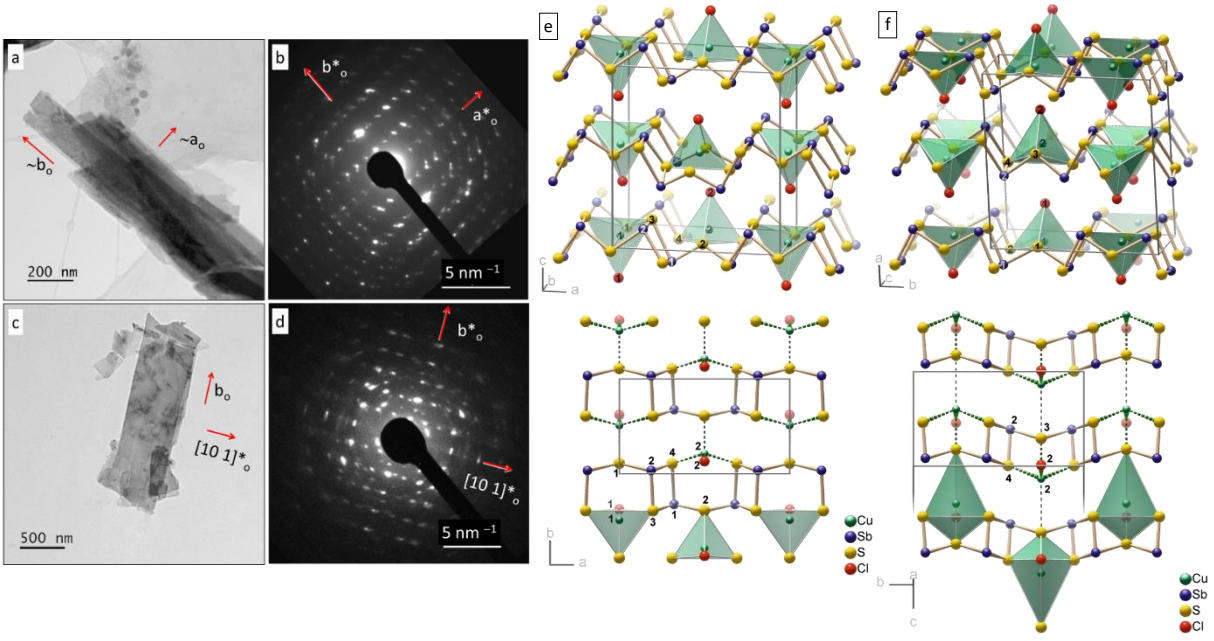

Figure 1: Sonicated $Cu(Sb_2S_3)Cl$ particles observed by TEM (a,c) and respective diffraction patterns (b,d). Right: Crystal structure of the orthorhombic (e) and (f) monoclinic form.

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Twist Angle Dependent Enhancement of Interlayer Exciton Emission in TMDC Heterotrilayer

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Abstract

Transition metal dichalcogenides (TMDC) heterostructures (HS) obtained by stacking two or more different TMDC monolayers (ML) are a new class of promising semiconducting materials. Due to their type-II band alignment, TMDC HS tend to host spatially indirect interlayer excitons (IX), where electrons and holes are located in the conduction and valence bands of the different layers. Particularly, the IX formed in a $WSe_2/MoSe_2$ heterobilayer are very fascinating as they showcase strong permanent out-of-plane dipole moment and moiré potential resulting from the twist angle dependent moiré superlattice [1], providing an intriguing and tunable platform for many-body physics investigations [2].

Interestingly, the IX emission can be manipulated by changing stacking order and the twist angle between the constituent layers [3][4]. Here we investigate for the first time the twist angle dependent enhancement of interlayer exciton emission in $WSe_2/WSe_2/MoSe_2$ heterotrilayer (HTL) systems prepared by using dry-transfer method. The IX exciton forming at the heterojunction in the HTL region exhibits a up to 10-fold increase in PL yield compared to HBL region on the same sample. To shed more light on the enhancement of the IX emission, we performed detailed DFT calculations and effective modelling of the low energy IX states. Focusing on the high symmetry stackings of the moiré superlattice, our calculations provide significant insight about interaction between all three layers that contributes to the formation and relaxation of new IX states in the HTL system. Our fundamental study of excitons in HTL system deepens the current understanding of physics of twisted TMDC heterostructures and paves the way for further experiments, theoretical work and applications in optoelectronic devices such as TMDC-based nanolasers.

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Creation of graphene quantum dot nanoarrays in van der Waals heterostructure

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Abstract

Quantum dot nanoarrays on graphene have generated interest for their ability to mimic the moiré potential observed in twistronics. While the moiré potential is sensitive to the twist angle, we present a method to periodically modulate the graphene potential by stacking graphene on 1T/2H-$NbSe_2$. The doping effect from the charge density wave of 1T-$NbSe_2$ allows for the formation of quantum dot nanoarrays independent of the periodically twist angle. Using scanning tunneling spectroscopy, we visualized the atomic-scale electronic structure of graphene/1T/2H-$NbSe_2$ samples with two different twist angles. These nanoarrays consistently follow the 1T-$NbSe_2$ charge density wave superlattice, independent of the twist angle. Furthermore, the interplay between the moiré potential and the quantum dot nanoarrays reveals novel phenomena: a larger twist showed a triangular mesh superlattice of unbounded states, while a smaller angle showed stripe patterns, breaking the C6 symmetry. By varying the coupling strength between the tip and the sample, we find that the lifetime of electron in the unbound states is longer than in the bound states. Our research paves the way for the fabrication and manipulation of quantum dots nanoarrays, extending beyond graphene to other 2D van der Waals heterostructure that are not limited by twist angle.

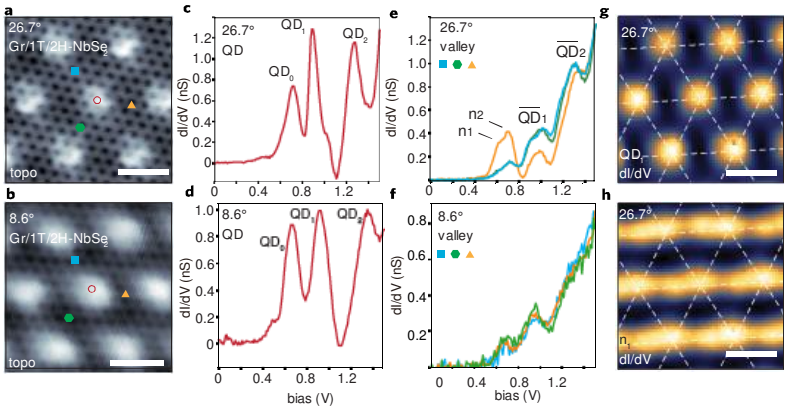

Figure 1: **a,b** topography of graphene on 1T/2H-$NbSe_2$ with various twist angle; **c,d** d*I*/d*V* spectra acquired on the QD; e,f d*I*/d*V* acquired on the valley positions as indicated in **a** and **b** respectively; **g, h** d*I*/d*V* grids of Gr/1T/2H-$NbSe_2$ with twist angle of 26.7° (scale bar = 1nm).

MOCVD-grown Topological Insulator Sb_2Te_3 Thin Films

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Abstract
Antimony telluride (Sb_2Te_3) is a narrow band gap p-type semiconductor with a layered crystal in which 5 atom thick Te–Sb–Te–Sb–Te sheets, called quintuple layers, are weakly coupled by van der Waals bonds. This crystallographic structure leads to a high thermoelectric figure of merit, hence, Sb_2Te_3 is widely used as a low-temperature thermoelectric material, especially, in mobile and wireless electronics. Furthermore, its topological insulating properties has captivated the attention of researchers worldwide. Topological insulators (TIs) feature a band gap in their bulk while exhibiting conducting surface states that form a spin-polarized Dirac cone similar to the dispersion diagram of graphene. The novel properties of TIs have given rise to various applications in the fields of electronics, spintronics, and quantum communications.

At CNR-IMM, we have achieved quasi-epitaxial Sb_2Te_3 thin films via metalorganic chemical vapor deposition (MOCVD) grown on large-area Si(111) substrates [1]. We have studied the magnetoresistance of these samples at cryogenic temperatures that reveal the existence of topological insulating properties [2]. We are actively conducting research on optimizing the deposition processes as well as utilizing Sb_2Te_3 thin films in different structures and applications.

Figures

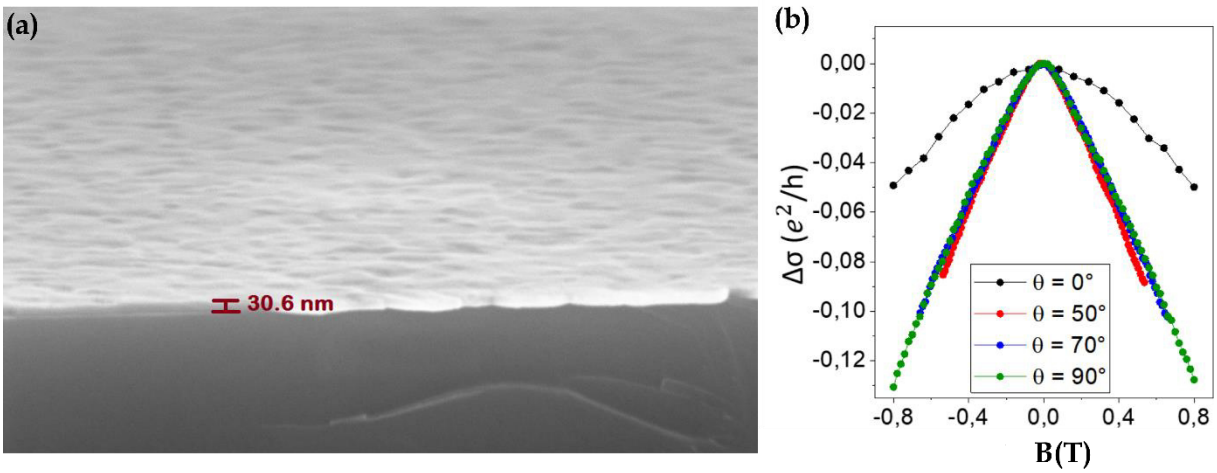

Figure 1: (a) Scanning electron microscopy (SEM) of a cross-section of a Sb_2Te_3 thin film on a silicon substrate. (b) Magnetoconductance curves at 5.5 K with the magnetic field applied at different angles with respect to the surface of Sb_2Te_3 thin film. The non-parabolic shape of the curves is a signature of topological insulating properties.

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Magnetic configuration of MPS_3 and MPS_4 (M= Cr, Mn, Fe, Co, Ni)

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Abstract
Magnetic van der Waals materials, such as transition metal phosphorous chalcogenides MPS_3 and $CrPS_4$ (M = Mn, Fe, Co, and Ni), offer potential for spintronic applications due to their wide band gap (1.2 - 3.5 eV) [1] and efficient light absorption. While both belong to the C2/m space group, they differ in magnetic ordering, with MPS_3 preserving antiferromagnetic (AFM) ordering [1] and $CrPS_4$ changing from AFM to ferromagnetic (FM) in the monolayer limit [2]. However, the mechanism and role of ligand field theory and exchange interaction in these materials are still unclear, leaving room for further research on the magnetic states that may arise in $FePS_4$, $CoPS_4$, $MnPS_4$, and $NiPS_4$. We studied the stability and electronic properties of the MPS_4 family using DFT, focusing on magnetic properties. We used the GGA+U approach with Dudarev formalism [3] for the magnetic structure, testing different values for U. Phonon spectra were obtained using PHONOPY with interatomic force constants calculated by VASP using DFPT and finite differences.

First, we studied $CrPS_4$, and with all the tested functionals showed that the ground state is FM and has a magnetic moment of 3.0 μB/magnetic atom, and are in agreement with the literature, in which the magnetic state ground state is FM and magnetic moment of 2.8 μB/magnetic atom [4]. The best result with experimental data was obtained without U for the functional considered, so for $CrPS_4$ is unnecessary to consider the U parameter to get the correct lattice parameter or magnetic ground state. For $FePS_4$, the magnetic ground, the electronic properties, and the dynamical stability depend on the functional and U used. Usually, the comparison with experimental data, such as the band gap, indicates which value of U to use. In this case, it is impossible since $FePS_4$ has yet to be synthesized.

In conclusion, our study of $CrPS_4$ confirmed the FM ground state and magnetic moment found in previous literature. The magnetic ground state and the electronic properties depend on the U parameter, so comparing with the experimental data or using other methods, such as hybrid functional or the calculation by first-principles calculation, are essential to describe the magnetic properties of MPS_4.

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Contact patterning for 2D materials using thermal scanning probe lithography

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Abstract
Two-dimensional materials (2DMs) have gained attention in electronic devices due to their ultrathin nature and the ability to steer and modify their electron and hole conduction. These properties can be used in the development of novel electronic devices. But the recurring challenge of fabricating 2D devices is the fragility of the active layer of the 2DMs [1].

The conventional lithography techniques for metal electrode patterning used for 2D devices are electron beam lithography (EBL) and optical lithography (UV). However, these strategies have been demonstrated to have negative impacts on devices [2][3]. On the other hand, thermal scanning probe lithography (t-SPL) uses a heated tip to create high-resolution patterns, proving a well-suited and radiation-free patterning for the 2DMs [4],[5]. Typically, polyphthalaldehyde (PPA) is used as a resist since it thermally decomposes into volatile monomers above 150°C.

This work involves fabricating 2D devices, e.g., tungsten selenide (WSe2) based field effect transistors, by patterning their contacts using the t-SPL enabled by the commercially available system NanoFrazor. This helps the performance due to its non-invasive patterning principle that helps avoid or minimize damage compared to EBL and UV-based structuring techniques.

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Electrically Controlled charge qubit in van der Waals heterostructure: From ab initio calculations to tight-binding models

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Abstract
Quantum computing has the potential to revolutionize fields that depend on intensive computational applications, such as drug development and disease prediction simulations, materials' design, machine learning, big data, and cybersecurity. The key component of quantum information theory is the qubit, which utilizes the principles of quantum superposition to simultaneously represent both 0 and 1 values, in contrast to classical bits, which can only represent one value at a time. Several different approaches to physically implementing qubits have been suggested [1]. Recently, a qubit implementation for quantum computing through gated van der Waals (vdW) heterostructures as charge qubits has been proposed [2], here named vdW qubits. It explores the spatial superposition of electrons from the individual layers by studying the orbital composition of the bands as a function of the gate field. The proposal provided a new perspective in the area, given the extensive list of possible combinations of two-dimensional (2D) materials.

In this work, we investigate the structural and electronic properties of twenty 2D transition metal dichalcogenides within the Density Functional Theory (DFT). Those layers with optimal energy level alignment were selected to form the vdW qubits. To reduce the computational cost, a Tight-Binding (TB) approach is built from *ab initio* calculations, where the basis of atomic orbitals is obtained via Maximally Localized Wannier Functions (MLWF) from the previous DFT calculations. Our model, corroborated by DFT calculations, enabled the discovery of novel layered material combinations, offering new perspectives for new host heterostructures for vdW qubits implementation. We further analyze the dynamical properties of heterostructures hosting these qubits by constructing nanoribbons using the *ab initio* tight-binding model and the Kwant software. Electronic properties, including dispersion relation, densities of states, and currents for different nanoribbons configurations (edge and width) made out of the individual layer components comprising the heterostructures are investigated. This investigation aims to provide insight into the potential splitting of the wave packet propagated within the material, demonstrating that hybridization enables electron transmission between different layers, giving valuable understanding into qubit viability and future experimentation.

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Structure-Imposed Electronic Topology in Edged-Patterned Zigzag Graphene Nanoribbons

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Abstract

Edge-patterned zigzag graphene nanoribbons (ZGNR) are a family of graphene nanoribbons with interesting electronic and topological properties.[1] In our work, we focus on two classes of structures: cove-edged ZGNR (ZGNR-C) and gulf-edged ZGNR (ZGNR-G). They are derived from pristine ZGNR by removing carbon atoms from the zigzag edges in a periodical manner, then saturating the ribbons with hydrogen atoms to maintain the trivalency of the sp^2 carbon atoms. As shown in Figure 1, their structure can be described uniquely using the four structural parameters N, M, a, b.

In our previous work [2], we demonstrated that the electronic state and topological properties of ZGNR-C can be classified for all structural parameters using simple rules, thus showing a direct structure-electronic structure relationship. We expanded this description to include the more general structure type of ZGNR-G. We find that these can – identical to ZGNR-C – also be classified as either metallic, topological, or trivial semiconductors depending on their structural parameters. Moreover, unlike ZGNR-C, there is no steric repulsion between hydrogen atoms at the edges, making ZGNR-G perfectly planar systems. This makes them better candidates for on-surface synthesis and application in electronic devices. Hence, we investigated their properties with the tight-binding (TB) method and density functional theory (DFT) and demonstrated possible structures, including hetero-junctions, for experimental considerations.

Figures

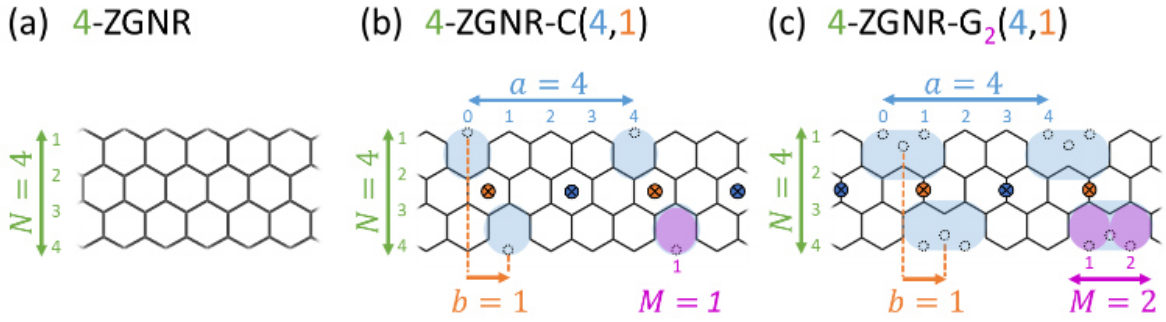

Figure 1: Schematic representations of (a) zigzag graphene nanoribbon (ZGNR), (b) cove-edged ZGNR (ZGNR-C) and (c) gulf-edged ZGNR (ZGNR-G). Width N, gulf size M, gulf distance a, and offset b are structural parameters. Orange and blue cross dots label the two distinct inversion centers.

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Excitonic features in an anisotropic ReS_2/WSe_2 heterostructure

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Abstract

Anisotropic two-dimensional (2D) materials, such as Rhenium disulfide (ReS_2), have emerged as a promising class of materials with polarized excitonic resonances. In this study, we present a novel 2D layered heterostructure composed of a monolayer of Tungsten diselenide (WSe_2) and a few layers of ReS_2 [1]. By employing polarization-resolved luminescence measurements, we reveal the presence of two additional polarization sensitive exciton peaks in ReS_2, in addition to the conventional exciton resonances X1 and X2[2]. Additionally, we observe two charged excitons (trions) in ReS_2, each exhibiting a binding energy of 18 meV and 15 meV, respectively. Intriguingly, the bi-excitons of WSe_2 [3] exhibit polarization sensitivity and acquire polarizing properties from the underlying ReS_2 layers, which act as patterned substrates for the top layer. Our research findings aim to harness the potential of spectroscopic techniques to manipulate various excitonic species, thereby opening avenues for advancements in optoelectronic and quantum photonics technologies.

Figures

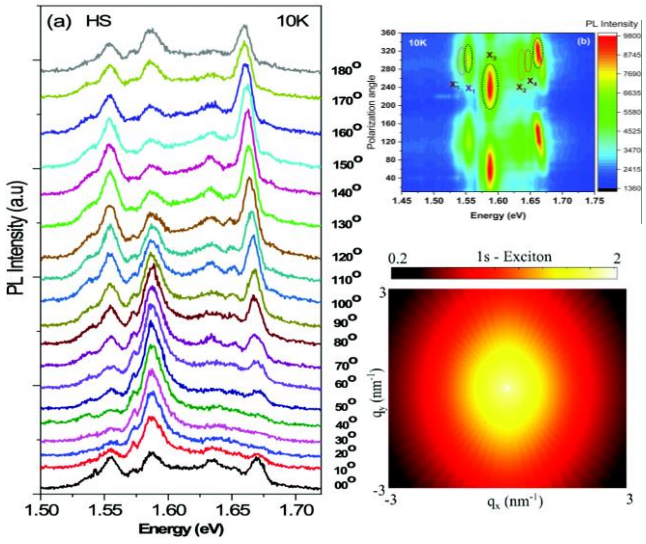

Figure 1: (a). Polarization-resolved PL spectra of the WSe_2/ReS_2 heterostructure at 10 K. (b). 2D contour plot of PL spectra with polarization angle (θ). (c) Square modulus of excitonic wave functions $|\varphi^{n}_{qx,qy}|^2$ for n = 0 (1s exciton).

References

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Tailoring the properties of the two-dimensional vdW materials.

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Abstract

By tuning the properties of materials, new discoveries can be made in fundamental science and pave the way for their practical applications. Emerging 2D materials like graphene offer an array of chemical and physical properties that can be further improved by fine-tuning their intrinsic properties. Among the many ways to achieve this, strain engineering is a promising technique due to the unique mechanical properties of these materials and their sensitivity to even the slightest perturbations. My work focuses on adopting strain engineering techniques to tune the properties of 2D materials. Additionally, I aim to address the development of sample preparation techniques, related applications, and the effects of biaxial strain on their electronic structures, phonon scattering, excitation dynamics like exciton funneling, and more.

References

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