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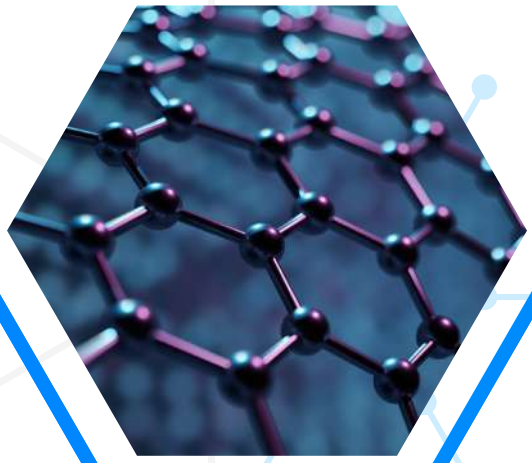
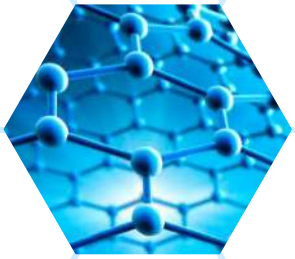
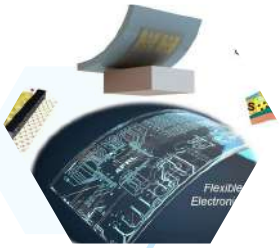
RECENT PROGRESS IN GRAPHENE AND 2D MATERIALS RESEARCH

20-23 NOVEMBER 2023 | VENUE: THE LALIT ASHOK BENGALURU







ABSTRACT BOOK

CONFERENCE MANAGER

GHA CONFERENCES

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MONDAY, 20 November, 2023		
Registration Opens: 08:00		
Welcome Note: 8:50-9:00, Grand Ballroom (GBR)		
Session 1A, GBR, Session Chair: Arindam Ghosh		
1A-1	09:00-09:30	**[Keynote] Ajay Sood** Insights into Quantum Topological Materials using Ultrafast Time Resolved Second Harmonic Generation
1A-2	09:30-10:00	**[Invited] Ajay Soni** Multibody Interactions and Symmetry Breaking Across the Charge Density Wave Transition of Transition Metal Dichalcogenides
1A-3	10:00-10:15	**[Contributed] Medha Dandu** Unveiling the spatial correlations of moiré excitons in WS2/WSe2 through hyperspectral monochromated EELS
1A-4	10:15-10:30	**[Contributed] Sourabh Jain** Excited-state trions: parallels between van der Waals semiconductors and 2D quantum wells
Session 1B, Lalit 1-2, Session Chair: Kausik Majumdar		
1B-1	09:00-09:30	**[Invited] Vinod Menon** Strong light-matter interaction in van der Waals materials
1B-2	09:30-10:00	**[Invited] Sajal Dhara** Towards Realization of Non-Hermitian PT-symmetry in Microcavity Exciton-Polaritons
1B-3	10:00-10:15	**[Contributed] Tamaghna Chowdhury** Tensile strain induced brightening of momentum forbidden dark excitons in monolayer WS2
1B-4	10:15-10:30	**[Contributed] Sarthak Das** Electrical control over valley polarization for charge excitonic species
Session 1C, Lalit 3-4, Session Chair: Atindra Nath Pal		
1C-1	09:00-09:30	**[Invited] Yoshihiro Iwasa** Nonlinear transport and diode effect in transition metal dichalcogenide superconductors
1C-2	09:30-10:00	**[Invited] Erik Henriksen** Probing graphene with infrared light, and infrared light with graphene
1C-3	10:00-10:15	**[Contributed] Radhika Soni** Planar tunneling in twisted moiré heterostructures

1C-4	10:15-10:30	**[Contributed] Nasir Ali** Quantum Criticality of Ambipolar Metal-Insulator Transitions in Black Phosphorus
Inauguration Ceremony: 10:30-10:45, Grand Ballroom (GBR), Special Invitee- Bharat Ratna Prof. CNR Rao		
COFFEE BREAK, 10:30-11:00		
Session 2A, GBR, Session Chair: Ashish Arora		
2A-1	11:00-11:30	**[Keynote] Young Hee Lee** Van der Waals Layered Magnetic Semiconductors
2A-2	11:30-12:00	**[Invited] Andras Kis** Exciton Manipulation and Transport in 2D Semiconductor Heterostructures
2A-3	12:00-12:15	**[Contributed] Shreya Paul** Stark shift of anisotropic excitons in few-layer ReS2
2A-4	12:15-12:30	**[Contributed] Santosh Kumar** Single photon emitters in monolayer WS2 emitting in the visible spectral range
Session 2B, Lalit 1-2, Session Chair: Debjani Karmakar		
2B-1	11:00-11:30	**[Invited] Abhishek K. Singh** Machine Learning Framework for Discovery of Novel Materials
2B-2	11:30-12:00	**[Invited] Hridis Kumar Pal** Effect of nonlocal interlayer hopping in twisted bilayer graphene
2B-3	12:00-12:15	**[Contributed] Debasis Dutta** Intrinsically nonreciprocal bulk plasmons in noncentrosymmetric magnetic heterostructures
2B-4	12:15-12:30	**[Contributed] Pilkyung Moon** Quasicrystalline Resonant States and Geometry of van der Waals Quasicrystals
Session 2C, Lalit 3-4, Session Chair: Adarsh K. V.		
2C-1	11:00-11:30	**[Invited] Prasana Kumar Sahoo** Electronic Grade 2D Lateral Heterostructures and Devices
2C-2	11:30-11:45	**[Contributed] Pinaka Pani Tummala** Vapor transport deposition of Transition Metal Tellurides (TMTs) and Ultra-Thin Tellurium nanosheets through Simulation-Guided Tellurization
2C-3	11:45-12:00	**[Contributed] Martin Wilken** Single source precursor pathway towards CVD of MoS2 thin films
2C-4	12:00-12:15	**[Contributed] Naresh Shyaga** Synthesis of Pristine and Nitrogen-Doped Graphene using solid precursors via CVD for SERS application

2C-5	12:15-12:30	**[Contributed] Jean-Pierre Glauber** Exploring gas phase processed tungsten sulfides for gas sensing applications
LUNCH BREAK: 12:30-14:00		
Poster session 1, Exhibition Hall		
P1	14:00-15:30	**Poster Session**
COFFEE BREAK: 15:30-16:00		
Session 3A, GBR, Session chair: Anindya Das		
3A-1	16:00-16:30	**[Keynote] Andrea Ferrari** Layered materials as a platform for quantum technologies
3A-2	16:30-17:00	**[Invited] Manish Chhowalla** Ultra-clean contacts on 2D semiconductors
3A-3	17:00-17:15	**[Contributed] Debasish Biswasray** Contact resistance for Metal-TMD heterostructures: Ab initio study
3A-4	17:15-17:30	**[Contributed] Bikas C. Das** Multifunctional Memristors Based on Two-Dimensional Layered Materials
Session 3B, Lalit 1-2, Session chair: Vidya Kochat		
3B-1	16:00-16:30	**[Invited] Young-Woo Son** Roles of interactions in layered materials
3B-2	16:30-17:00	**[Invited] Johannes Lischner** Electrons, excitons and phonons in moiré materials from atomistic simulations
3B-3	17:00-17:15	**[Contributed] Devarshi Chakrabarty** Exceptional Points in a Non-Hermitian anisotropic exciton-polariton pair system
3B-4	17:15-17:30	**[Contributed] Anuj Kumar Singh** Engineering of excitonic lineshape and valley dynamics in two dimensional semiconductors using low cost strain tuning
Session 3C, Lalit 3-4, Focus session on Startups and Hiring, Session Chair: U. Chandni		
3C-1	16:00-16:20	**Manjunath Jyothinagar, KAS Technologies**
3C-2	16:20-16:40	**Gayathri HN, Quan2DTechnologies Pvt. Ltd.**
3C-3	16:40-17:00	**Deep Talukdar, Cryo Nano**
3C-4	17:00-17:20	**Solomon Jones, Terracarb Pvt. Ltd.**
3C-5	17:20-18:00	**Networking Session**

Insights into Quantum Topological Materials using Ultrafast Time Resolved Second Harmonic Generation

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Ever since the discovery of graphene, optical spectroscopies, in particular Raman and time resolved spectroscopies, both linear and nonlinear, have played key roles in probing quantum materials, including 2D systems. In this talk, I will focus on our recent results related to the second harmonic generation (SHG) from 2D transition metal dichalcogenides [1, 2]. The lessons learnt from our recent time-resolved SHG studies from topological insulator Bi_2Te_3 [2] and type I Weyl semimetals (WSM) [3] will be useful for understanding the topological type II WSM TMDs.

(1) K.P. Bera, D. Solanki, S. Mandal, R. Biswas, T. Tanaguchi, K. Watanabe, V. Raghunathan, M. Jain, A.K. Sood and A. Das; Twist angle dependent phonon hybridization in WSe_2/WSe_2 homobilayer (2023).

(2) Aindrila Sinha, K.P. Mithun and A.K. Sood; Ultrafast SHG in type II Weyl semimetallic phases of $MoTe_2$ and WTe_2 (2023).

(3) Aindrila Sinha, K.P. Mithun and A.K. Sood, Time-resolved SHG in topological insulator Bi_2 Te_3: Competing contributions from Dirac surface states, surface photovoltage and band bending, ACS Photonics (2023).

(4) K.P. Mithun, Aindrila Sinha, C. Shekhar, C. Felser and A.K. Sood, Shift current dominated ultrafast dynamics of SHG in Type I Weyl semimetals (2023).

Multibody Interactions and Symmetry Breaking Across the Charge Density Wave Transition of Transition Metal Di Chalcogenides

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ABSTRACT

Atomically thin materials have displayed a paradigm shift for understanding of physical and electronic properties because of quantum size effects, broken symmetry and dielectric screening.[1-4] One of the interesting quantum phenomena is Charge density wave (CDW), where the periodic modulation of the electronic charge density is accompanied by the lattice distortion with high anharmonicity.[4-5] The reconstruction of the lattice leads to folding of Brillouin zone along with emergence of collective modes and enhanced multi body interactions.[4, 6, 7] The talk will discuss the thickness dependence of CDW in layered 2H-TaS_2 and multiphonon interactions accessed through spectroscopy and electrical transport. Bulk 2H-TaS_2 endures a CDW transition at ~ 76 K, however the onset of CDW instability in can exist up to 200 K due to breaking of translational and center of inversion symmetry. The transition temperature has inverse relation with the thickness of atomically thin layers. [6-7]

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Unveiling the spatial correlations of moiré excitons in WS_2/WSe_2 through hyperspectral monochromated EELS

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Twisted stacks of layered materials such as transition metal dichalcogenides (TMDs) have emerged as a promising platform for the bottom-up design of artificial superlattices offering control over the arrangement and interactions of quasi-particles[1]. Nanoscale moiré superlattices of TMDs can enable programmable excitonic emitter arrays for quantum optoelectronic applications[2,3]. The spatial and spectral modulations of excitons in the moiré superlattice depend on the lattice mismatch and twist angle across the individual layers, which affect the electronic states through atomic reconstruction and interlayer hybridization. Conventional optical spectroscopy reveals multiple spectral resonances of moiré excitons in aligned WS_2/WSe_2 bilayers[4] from an ensemble of moiré supercells. However, this limited spatial resolution lacks insights into the nanoscale excitonic phenomena of moiré superlattices[5]. This work uses scanning transmission electron microscopy (STEM) to perform hyperspectral imaging of intralayer moiré excitons in WS_2/WSe_2. Using a sub-nanometer monochromated (~10 meV) probe, we acquire fast and serial low-loss electron energy loss spectroscopy (EELS) and annular dark field (ADF) images simultaneously. These correlated data provide insights into the spatial variation of exciton features at the length scale of a moiré supercell in R-stacked WS_2/WSe_2 samples, revealing the interplay between interlayer hybridization and atomic reconstruction. These observations help us better understand exciton physics in the moiré landscape of twisted bilayers.

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Excited-state trions: parallels between van der Waals semiconductors and 2D quantum wells

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Charged excitons, also known as trions, have been predicted in solids since 1958[1]. The ground state of trions has been experimentally observed in both monolayers of semiconducting transition metal dichalcogenides (TMDCs) and 2D quantum wells (QWs)[2,3]. While the excited state of trions has been detected in monolayer of WS_2[4] and WSe_2[5], it has not been observed in spectra of QWs. This is because ground-state trion's binding energy and oscillator strength in QWs are an order of magnitude smaller than TMDCs[2]. Consequently, these parameters for the excited-state trions are expected to be even smaller, making their experimental detection extremely challenging. Furthermore, it is not established theoretically if the excited-state trions in QWs are bound states at all, or not.

In parallel with TMDC monolayers, we report experimental observations of an excited-state of a trion in a 4.2 nm thin unintentionally-doped GaAs/AlGaAs QW[6]. Using the highly-sensitive magneto-optical Kerr effect (MOKE) spectroscopy, we are able to clearly identify spectral features corresponding to the doubly-excited 2s trion. Application of an out-of-plane magnetic field enhances the binding energy and oscillator strength of the 2s trion, which enables us in its detection. Careful line shape modelling based on the transfer-matrix method is used for the data analysis. The opposite circular-polarization trends observed in the 2s exciton and 2s trion confirm our identification. Our experimental data suggests that this excited-trion state is most likely unbound in the absence of a magnetic field.

Our work represents first observation of an excited-state of a trion in a 2D quantum well and solves the long-standing puzzle regarding their detection. It is expected to open new directions in the theoretical and experimental research of Rydberg states of trions.

References

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Strong light-matter interaction in van der Waals materials

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Strong light-matter interaction results in the formation of half-light half-matter quasiparticles called polaritons that take on the properties of both its constituents. In this talk, I will first introduce polariton formation in van der Waals (2D) materials and specifically, exciton-polaritons in 2D semiconductors [1]. Following this, we will discuss Rydberg polaritons [2] and dipolar polaritons [3] to realize highly nonlinear interactions motivated by the need for single photon nonlinearity. Finally, we will discuss our recent work on coupling of magnetically correlated excitons in van der Waals magnets with cavity photons [4, 5]. The prospects for modifying magneto-optical response and controlling the interaction between excitons, photons and magnons will also be discussed.

References

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Towards Realization of Non-Hermitian PT-symmetry in Microcavity Exciton-Polaritons

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Abstract: Microcavity exciton-polaritons offer a promising platform for quantum optics and condensed matter physics, making them a potential candidate for quantum technologies. Recently, significant attention has been drawn towards understanding the non-Hermitian topology of exciton-polaritons in the framework of cavity quantum electrodynamics. One of the prominent platforms for realizing non-Hermitian exceptional points in polariton bands is anisotropic exciton-polaritons, where light-matter interaction can be tuned with the polarization of the probe beam. Exceptional points are degeneracies of non-Hermitian polariton bands realized in the momentum space due to anisotropic light-matter coupling originates from structural anisotropy. In this talk, I shall present our recent work on anisotropic exciton-polaritons of few layer ReS_2 embedded in an optical microcavity offering two sets of topologically non-trivial polaritons with emergence of exceptional points. Furthermore, I shall present a unique approach towards the realization of quantum PT-symmetry resulting in polariton-Raman laser in such non-Hermitian system. It will be shown that the unique property of the anisotropic two-dimensional material enabling us to achieve this result is the existence of Raman active phonon modes undergoing stimulated resonant Raman scattering between polariton modes.

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Tensile strain induced brightening of momentum forbidden dark excitons in monolayer WS_2

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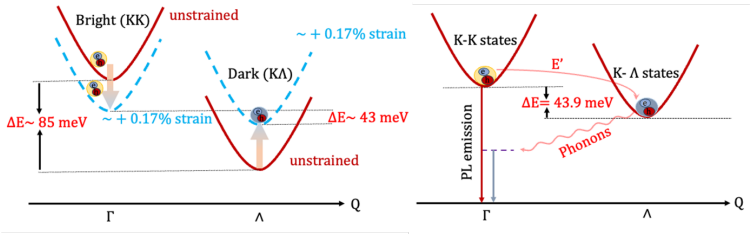
Transition metal dichalcogenides (TMDs) are known for their novel optical properties. The monolayer (ML) TMDs have strong in-plane covalent bonds and therefore they can endure strain of a few percentages, which significantly effects the electronic band structure, electron-phonon coupling etc. Therefore, strain is a very effective tool for modifying excitonic landscape of TMDs. The calculated electronic band structure of ML WS_2 show the existence of various excitonic species. There is possibility for the formation of indirect intervalley exciton between a hole at valence band minima at K point and an electron at the conduction band minima at Λ point. But because of large momentum mismatch, they require assistance of phonons for their formation. On optically exciting a coherent exciton population at Γ-point (in terms of exciton center of mass coordinates), the K-K excitons can then scatter to the Λ point, assisted by available phonon mode to form K-Λ excitons. However, due to a large energy splitting between the exciton states at Γ and Λ points the scattering channel is not always available and hence we don't see any optical signature of K-Λ exciton. That's why the K-Λ excitons are called 'dark'. K-Λ exciton is the excitonic ground state for W-based TMD materials, therefore they play an important role on the exciton-dynamics of the system.

In this work we brighten the K-Λ 'dark' exciton by applying tensile strain on CVD grown ML WS_2 by placing the MLs on nanotextured substrate prepared by block-copolymer lithography. We observe a new peak at low energy in temperature dependent photoluminescence (PL) spectroscopy measurements for a particular value of strain ($\sim$0.17%), while this new peak is not observed for other values of strain and unstrained sample. Using excitation power dependent studies, we confirm this to be a dark exciton peak. From phenomenological analysis of temperature dependent PL spectra in case of $\sim$0.17% strained sample we find the average phonon energy to be $\sim$ 43 meV which is close to the energy of the in-plane phonon mode E'. From DFT calculations, we find the dark-bright energy splitting (ΔE) to be $\sim$ 85 meV in case of unstrained ML WS_2 while in $\sim$0.17% strained sample, ΔE is estimated to be $\sim$ 44 meV. This energy gap in strained sample ($\sim$0.17%) is now accessible to the E' phonon mode and therefore the bright K-K excitons can now scatter to the Λ valley to form the dark K-Λ excitons. The K-Λ excitons can decay to a virtual state at Γ point inside the light cone, from where they can decay radiatively resulting in PL. The strong exciton-phonon coupling is further confirmed by anomalous behavior of the E' phonon mode in temperature dependent Raman spectroscopy. The value of strain is also confirmed experimentally by softening of Raman modes.



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Electrical control over valley polarization for charge excitonic species

Sarthak Das[1], Ding Huang[1], Ivan Verzhbitskiy[1], Chit Siong Lau[1], Kenji Watanabe[2], Takashi Taniguchi[3], and Kuan Eng Johnson Goh[1,4,5]

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Monolayer transition metal dichalcogenides (TMDs) have unique property of valley-contrasting spin splitting, which allows the spin of an electron/hole locked to its valley. This makes monolayer TMDs ideal for studying valley physics, as it allows us to control the valley polarization of excitons [1]. However, the quantum states of excitons are easily affected by environmental noise, which can lead to the loss of quantum information. The electrical control of excitons is also difficult and so its valley properties, as they are charge neutral. However, the monolayer TMDs can host multi-particle excitonic states by capturing additional electrons with high binding energy due to its dimensionality. In this work we investigated the possibility of electrically control the valley polarization of charged excitonic species, such as trions and quintons (charged biexcitons). We have also explored the valley properties of charged excitonic species by dynamic electrical modulation of its valley polarization. We have shown that the valley information can be protected in presence of enhanced scattering due to intervalley exchange interaction along with the q-space dispersion of the charged energy states hitherto unexplored. The valley polarization thus not only can be preserved but also can be modulated under the stochastic variation of the electrical environment. These results are important for the development of valleytronics [2,3], as they show that it is possible to control the valley polarization of charged excitonic species in a deterministic way. This could lead to the development of new devices that use valley polarization for quantum information processing.

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Nonlinear transport and diode effect in transition metal dichalcogenide superconductors

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Nonlinear transport in materials with broken inversion symmetry is recently attracting a significant interest in various aspect of transport properties. Superconductors are no exception. The nonreciprocal transport of intrinsic origin has been first found in gate-induced superconductivity in MoS_2 and WS_2 nanotubes, which are trigonal and polar in symmetry, respectively [1,2]. The nonreciprocal transport was detected by means of second harmonic resistance, which is an equivalent phenomenon to the second harmonic generation in optics. Later on, the DC rectification behavior, so call superconducting diode effect, was discovered [3,4]. Transition metal dichalcogenide based superconductors offer a unique platform of the study of nonlinear transport because of their trigonal unit layers with broken inversion symmetry. Here we report the nonreciprocal transport and superconducting diode effect in $PbTaSe_2$ with particular focus on the zero-magnetic field condition.

We first investigated the nonlinear anomalous Hall effect (NAHE), which is known to be driven by the Berry curvature dipole. We observed a NAHE both in the normal state and around the superconducting transition temperature, despite the absence of polar structure and the Berry curvature dipole. The NAHE signal in the superconducting state is two orders of magnitude larger than that in the normal state, in a similar manner to the nonreciprocal superconducting transport [5].

Despite a large number of reports in the superconducting diode effect either in intrinsic or extrinsic in origin, most of the reports have been on systems under magnetic field or proximitized with a ferromagnet, in other words, under broken time reversal symmetry [4]. Thus, the superconducting diode effect under zero magnetic field is still elusive. For investigation of intrinsic mechanisms of the superconducting diode effect, we believe that the measurement of symmetry dependent transport is highly crucial. We have measured the superconducting diode effect on unstrained $PbTaSe_2$, and found there is no zero-field superconducting diode effect, despite that it is symmetry allowed. In sharp contrast, we found that the zero-field the superconducting diode effect was induced in the strained $PbTaSe_2$. We discuss about the nonlinear superconducting transport from the viewpoint of symmetry.

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Probing graphene with infrared light, and infrared light with graphene

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Abstract:

Infrared magnetospectroscopy is used to explore the \nu=0 state in both mono- and bilayer graphene. In the latter, multiple transitions appear and disperse non-monotonically as a displacement field is applied perpendicular to the sheet. The results are consistent with the canted antiferromagnet but suggest the possibility of additional phase transitions between the CAFM and the fully layer polarized state. In separate experiments, we pursue a graphene-based single photon detector in the far-infrared, and discuss relevant thermal transport properties of monolayer graphene that make it a nearly ideal material for bolometry.

Planar tunneling in twisted moiré heterostructures

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The ability to exfoliate 2D materials from the bulk, such as graphene and hexagonal boron nitride (hBN), has allowed experiments demonstrating exceptional quantum mechanical phenomena, such as quantum tunneling, in low-dimensional systems. Several earlier investigations utilized a few atomic layers of hBN as the tunnel barrier to show how an electron can tunnel from a metal into a sheet of graphene or graphite [1-3]. Following theoretical predictions that graphene layers will be strongly coupled close to the so-called "magic" angles, where the low energy bands become extraordinarily flat, experiments have shown evidence of substantial correlations [4–7]. In this study, we employ the innovative technique of electron tunneling to investigate correlations in twisted moiré heterostructures. Twisted bilayer graphene was used to create vertical tunneling transistors, while tungsten diselenide (WSe2) was used as the tunnel barrier. Figure 1a depicts the device's schematic, and Figure 1b displays the tunneling conductance (dI/dV) as a function of the bias voltage (V_{DC}) and gate voltage (V_{TG}). In this session, I'll further detail how we have investigated correlations in the moiré bands at low temperatures using tunneling as a sensitive probe.

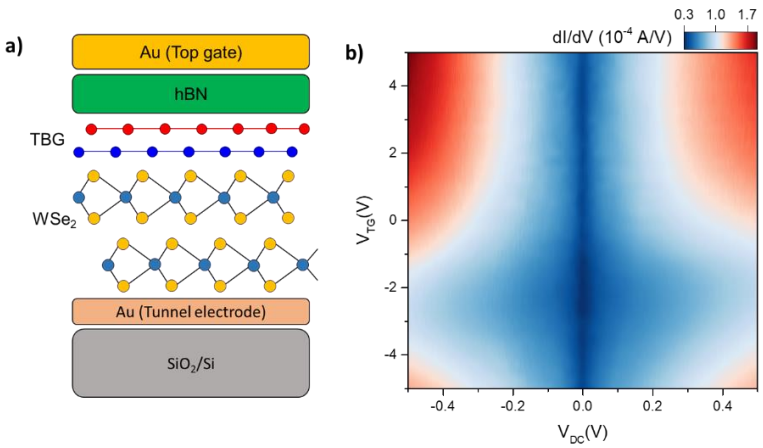

Figure 1 a. Schematic of the device **b.** Tunneling conductance (dI/dV) as a function of bias voltage (V_{DC}) and gate voltage (V_{TG})

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Quantum Criticality of Ambipolar Metal-Insulator Transitions in Black Phosphorus

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Quantum phase transition is an abrupt change in ground states of many-body systems owing to quantum fluctuations that facilitate exotic states and quantum critical behavior [1, 2]. Here, we report the density-driven metal-insulator transitions (MITs) in hole and electron regimes of black phosphorus (Figure 1). In the hole regime, Fermi liquid and *T*-linear behaviors have been found in the metallic phase and at the metal-insulator boundary, respectively. While in the electron regime, we observe the Fermi liquid behavior in deep metallic phase at low temperatures, and *T*-linear behavior at high temperatures from deep metallic phase to metal-insulator boundary. Further, we performed scaling analysis that supports the quantum criticality in hole and electron regimes. We observe asymmetric critical exponents around the MITs, which occurs from strong screening in metallic phase and conversely poor screening in insulating phase due to free carriers in hole and electron regimes. Finally, we discuss the impact of anisotropy on the critical exponents in metallic and insulating phases in the hole regime. Our study provides compelling evidence that ambipolar black phosphorus becomes a suitable system to study 2D MIT in hole and electron regimes in 2D systems.

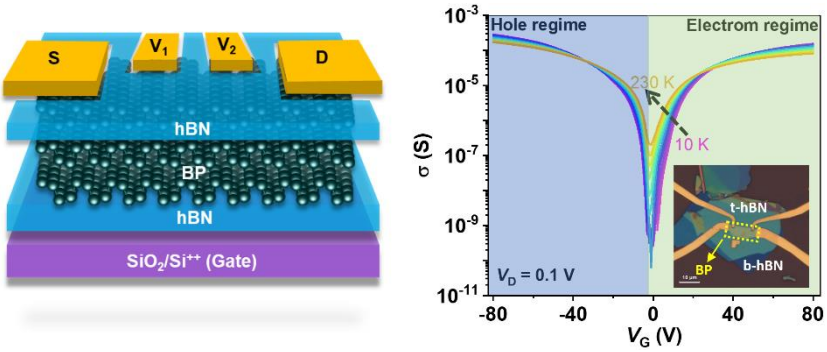

Figure 1. Observation of metal-insulator transitions in hole and electron regimes of black phosphorus.

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van der Waals layered magnetic semiconductors

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Ferromagnetism in van der Waals two-dimensional (2D) materials has been reported re cently. Intrinsic CrI_3 and $CrGeTe_3$ semiconductors reveal ferromagnetism but the Tc is still low below 60K. In contrast, monolayer VSe_2 is ferromagnetic metal with Tc abov e room temperature but incapable of controlling its carrier density due to metallic natu re. Difficulty arises from lack of right ferromagnetic semiconductors. Historically, dilut ed magnetic semiconductors (DMSs) have been introduced by doping the minute amou nt of magnetic dopant such as Mn, in III-V or II-VI semiconductors has been introdu ced as an alternative. Moreover, the long-range ferromagnetic order in doped diluted c halcogenide semiconductors has not been demonstrated at room temperature. The key r esearch target here is to realize the long-range order ferromagnetism, Tc over room te mperature, and gate tunability. In this talk, we introduce magnetic dopant, vanadium i n semiconducting WSe_2 and manifest Tc at room temperature and gate tunability at lo w doping concentration. This could be realized via strong spin orbit coupling and stro ng Coulomb interaction in van der Waals layered transition metal dichalcogenides, for example, WSe_2 layer. We further explore different doping concentrations including hig hly degenerate regime and demonstrate unconventional magnetic order by random teleg raph spin noises via interlayer coupling at low doping concentration limit and strange metal if time is allowed.

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Exciton Manipulation and Transport in 2D Semiconductor Heterostructures

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The discovery of graphene marked the start of research in 2D electronic materials which was expanded in new directions with MoS_2 and other layered semiconducting materials. They have a wide range of interesting fundamental properties and potential applications. New opportunities are enabled by the band structure of transition metal dichalcogenides (TMDCs) in which we could harness the valley degree of freedom for valleytronics and next-generation photonics. Long-lived interlayer excitons in van der Waals heterostructures based on TMDCs have recently emerged as a promising platform for this, allowing control over exciton diffusion length, energy and polarization. I will show here how by using MoS_2/WSe_2 van der Waals heterostructures, we can realize excitonic transistors with switching action, confinement and control over diffusion length at room temperature in a reconfigurable potential landscape. On the other hand, the weak interlayer interaction and small lattice mismatch in $MoSe_2/WSe_2$ heterostructures results in brightening of forbidden optical transitions, allowing us to resolve two separate interlayer transitions with opposite helicities and meV-scale linewidths. These have opposite helicities under circularly polarized excitation, either preserving or reversing the polarization of incoming light. By using externally applied electrical fields, we can control their relative intensities and polarization by different regions in the moiré pattern, characterized by different local symmetries and optical selection rules. Our more advanced excitonic devices now also offer the way to manipulate the motion of valley (spin) polarized excitons and to electrically control the size of the interlayer exciton dipole moment.

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Stark shift of anisotropic excitons in few-layer ReS_2

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Rhenium dichalcogenides are members of the 2D TMDC family which show anisotropic optical properties. Rhenium disulphide (ReS_2) has two different stable stacking orders, AA and AB. In this study, we investigate the effect of out-of-plane electric field on X_1 and X_2 excitons in AB stacked few-layer ReS_2. At a temperature of 4 K, we observed a quadratic Stark shift of 13 meV for both X_1 and X_2 excitons which enabled us to deduce the out-of-plane polarizabilities of X_1 and X_2 excitons ($(5.72 \pm 0.39) \times 10^{-8}$) D-m/V and ($(4.50 \pm 0.40) \times 10^{-8}$) D-m/V, respectively. Our findings highlight the pronounced confinement of the excitons which paves the way for future applications in optoelectronic devices.

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Single photon emitters in monolayer WS_2 emitting in the visible spectral range

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A van der Waals heterostructure/device containing an atomically-thin transition-metal dichalcogenide (TMD) as a single-photon emitting layer is emerging as an intriguing solid-state quantum photonic platform [1]. Various methods of strain engineering have been utilized for creating/inducing the quantum emitters in monolayer (ML) and few-layer TMDs at deterministic locations [2-4]. Here, we present a simple and cost-effective approach using the spin coating of silica nanoparticles for deterministically creating the spectrally isolated, energetically stable, and narrow-linewidth single-photon emitters in ML-WS_2. The emission wavelengths of these quantum emitters are in the visible spectral range where most commercially available single photon detectors work efficiently. We also demonstrate that the low-temperature annealing of this photonic heterostructure, containing ML-WS_2, in the vacuum is causing the removal of energetically unstable emitters and leading to the emission of single photons in a narrow wavelength range.

Furthermore, we show that the annealing-induced enhanced conformality of the light-emitting layer onto the nanoparticles is causing an enormous tensile strain in the light-emitting layer at the nanoparticle locations. We have estimated a local-strain of up to 1.2% in ML-WS_2. The work presented here may provide valuable insights into the quantum properties of 2D materials, which will have implications on the fundamental understanding and technological development of single-photon emitting heterostructures/devices for future quantum photonic technologies.

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Machine Learning Framework for Discovery of Novel Materials

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Data driven machine learning methods in materials science are emerging as one of the promising tools for expanding the discovery domain of materials to unravel useful knowledge. In this talk, the power of these methods will be illustrated by covering two major aspects, namely, development of prediction models and establishment of hidden connections. For the first aspect, we have developed accurate prediction models for various computationally expensive physical properties such as band gap, band edges and lattice thermal conductivity. The prediction model for band gap and band edges are developed on 2D family of materials -MXene, which are very promising for a wide range of electronic to energy applications, which rely on accurate estimation of band gap and band edges. These models are developed with GW level accuracy, and hence can accelerate the screening of desired materials by estimating the band gaps and band edges in a matter of minutes. For the lattice thermal conductivity prediction model, an exhaustive database of bulk materials is prepared. By employing the high-throughput approach, several ultra-low and ultra-high lattice thermal conductivity compounds are predicted. The property map is generated from the high-throughput approach and four simple features directly related to the physics of lattice thermal conductivity are proposed. The performance of the model is far superior than the physics-based Slack model, highlighting the simplicity and power of the proposed machine learning models. For the second aspect, we have connected the otherwise independent electronic and thermal transport properties. The role of bonding attributes in establishing this relationship is unraveled by machine learning. An accurate machine learning model for thermal transport properties is proposed, where electronic transport and bonding characteristics are employed as descriptors. I will discuss the application of ML in establishing the complex structure-property relations in alloys.

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Effect of nonlocal interlayer hopping in twisted bilayer graphene

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Twisted bilayer graphene (TBG) and other related moire heterostructures have emerged as a fascinating playground for exotic physics in recent years, thanks to their unusual band structures and extraordinary tunability. The long-wavelength theory describing TBG typically includes the effect of the spatially varying interlayer hopping in the local approximation. I extend the theory by including nonlocal interlayer hopping terms and study their consequence on the low-energy band structure and observable quantities.

Intrinsically nonreciprocal bulk plasmons in noncentrosymmetric magnetic heterostructures

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Nonreciprocal plasmonics is a rapidly growing research field owing to the direction-dependent propagation of light or quantum information and is an essential building block for photonic applications. In this presentation, I will demonstrate the emergence of intrinsically nonreciprocal bulk plasmon modes in noncentrosymmetric magnetic materials [1]. I will discuss how the quantum geometry of the Bloch states (e.g- quantum metric, metric connection) significant intrinsic nonreciprocity in bulk intraband and interband plasmon dispersion[2]. Finally, I demonstrate the existence of this new kind of nonreciprocal plasmons in twisted bilayer graphene heterostructures having a ferromagnetic ground state. Our study of nonreciprocal plasmon with a quantum origin opens a new avenue of optical manipulation at the nanoscale.

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Quasicrystalline Resonant States and Geometry of van der Waals Quasicrystals

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Quasicrystal is a unique form of solid matter which is ordered but not periodic. Although quasicrystals are expected to provide important insights into the atomic order at the interface between periodic crystals and amorphous, their electronic structures have been investigated mainly using inevitable approximations sacrificing a part of its characteristic symmetries. Recently, a new type of quasicrystal, "van der Waals quasicrystals", is realized by stacking two atomically-thin layers at specific configurations [1]. We developed a theoretical model that can precisely calculate the electronic structures of van der Waals quasicrystals and revealed the emergence of quasicrystalline resonant states [2].

In this talk, we first show that the quasicrystalline resonant states appear in more general configurations: any pair of square lattices with a relative twist angle of $\theta = 45°$ and any pair of hexagonal lattices with a relative twist angle of $\theta = 30°$, if and only if all the dominant interlayer interactions occur between the atomic orbitals that have the same magnetic quantum number [3]. This implies that not only the quasicrystal composed of the widely studied graphene but also those composed of transition metal dichalcogenides will exhibit the quasicrystalline states. Then, we show the quasicrystalline states in double moiré superlattices [4] and Eshelby-twisted multilayers, an infinite stack of atomic layers with a constant twist angle between them, [5], and show their optical selection rules. Finally, we discuss the geometry of van der Waals quasicrystals and show that the existence of the "precise center", which exhibits the highest rotational symmetry, is not guaranteed in these systems because of the difference of the cardinality between the sets of integers and real numbers [5].

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Electronic grade 2D Lateral Heterostructures and Devices

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There are enormous possibilities in combining diverse 2D materials for the unique design of ultra-smart and flexible optoelectronic devices, including transistors, and quantum emitters.[1] Considerable efforts have been devoted to the van der Waals hetero-integration of different 2D layered transition metal dichalcogenides (TMDs) to form vertical superlattices by transferring their exfoliated or as-grown flakes. On the other hand, 2D lateral heterostructure is possible only via direct growth, which can offer exciting opportunities for engineering the formation, confinement, and transport of electrons, holes, exciton, phonon, and polariton. Furthermore, the performance of most 2D heterostructure-based devices falls far below the predicted values owing to several intrinsic and extrinsic factors. These significant issues will be discussed.

We reported the direct fabrication of seamless, high-quality TMDs lateral heterostructures and superlattices in the chemical-vapor-deposition process, only changing the reactive gas environment in the presence of water vapor.[2-5] Our novel approach offers greater flexibility for the continuous growth of multi-junction TMDs lateral heterostructures, controlled 1D interfaces, alloying, and layer numbers. The extent of the spatial modulation of individual TMD domains and their optical and electronic transition characteristics across the heterojunctions are studied in detail. Electrical transport measurements revealed diode-like responses across the 2D lateral junctions and showed promising photodetection and electroluminescence properties at room temperature. Temperature-dependent photoluminescence from neutral exciton, trion, and defect-bound exciton provides a better understanding of the optical properties of these as-grown 2D lateral heterostructures. These studies will further supplement the quantitative evaluation of the optical and electronic qualities of various 2D heterostructures to develop more complex and atomically thin superlattices and exotic devices.

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Dr. P. K. Sahoo is an experimental condensed matter physicist with broad experience studying different low-dimensional materials. He obtained Ph.D. in Physics from Homi Bhabha National Institute (HBNI)- a grant-in-aided institute of the Department of Atomic Energy, Govt. of India. He spent several years at the State University of Campinas, Brazil; University of South Florida, USA; and University of Cambridge, UK, before holding the position at the Materials Science Centre, IIT Kharagpur. Dr. Sahoo's work covered various areas of nanomaterials that, including 2D materials and heterostructures (graphene and beyond), group III-V-based semiconductor nanowires, and sensors. His current research focuses on exploring and understanding exotic 2D materials and their heterostructures, which have fundamental and a wide range of technological implications for future optoelectronics. He exploits a combination of materials synthesis, heterostructuring, spectroscopic characterization, and device fabrication for physicochemical properties assessment.

Vapor transport deposition of Transition Metal Tellurides (TMTs) and Ultra-Thin Tellurium nanosheets through Simulation-Guided Tellurization

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Tellurium-based two-dimensional (2D) materials possess unique characteristics that show potential as useful materials in various technological fields, spanning from nano-electronics to thermoelectric and energy sectors.[1] Specifically, 2D transition metal ditellurides (TMTs) can display either semiconductor or metallic properties based on their crystal phase structure, namely trigonal prismatic or octahedral. Among TMTs family, molybdenum ditelluride ($MoTe_2$) shows significant attention due to its polymorphic nature from semiconductor to topological insulator and Weyl-semimetal. [1-3] Similarly, the electronic and optical characteristics of 2D mono-elemental form of Tellurium (known as Tellurene) are greatly influenced by both its allotrope form and number of layers. In the α-phase, the most stable allotrope form in bulk, the electronic bandgap ranges from 0.92 eV in monolayer state to 0.33 eV in the bulk state.[4] To date, considerable efforts have been devoted for synthesizing large area $MoTe_2$ suitable for the fabrication of devices to be integrated in different applications. From this point of view, a precise synthesis of phase-selected, uniform $MoTe_2$ is essential.[2][3] Among many growth methods, chemical vapor deposition (CVD) is a facile and promising way for synthesizing large scale $MoTe_2$ nanosheets.

In this work, we thoroughly elaborate on the large scale and accurate phase-controlled growth of $MoTe_2$ films and atomically thin tellurium by CVD methods, demonstrated a correlation between the concentration gradient of Te vapor and the deposited $MoTe_2$ morphology and coverage.[2] We also developed a finite element simulation model (FEM) to understand the influence of experimental parameters, such as the substrate orientation, on the structural, morphological, and physical properties of the so-grown materials. Taking the advantage of FEM simulation guided experiments, we demonstrated a feasible CVD route for large scale growth with controlled phase tuning strategies for obtaining 1T'(metallic), 1T'/2H, and 2H (semiconducting) $MoTe_2$ nanosheets via tellurization of pre-deposited Mo thin film.[2] We show a detailed study of the heterogeneous vapor-solid reaction between a e-beam pre-deposited molybdenum film and tellurium vapor, thus yielding a large area growth of $MoTe_2$ onto SiO_2/Si substrate. Here, $MoTe_2$ growth and its phase selection is mainly influenced by the involved kinetics, tellurium concentration and geometry configurations inside the CVD furnace. Further, we expand our simulation guided tellurization methodology to realize other TMTs such as $PtTe_2$, $NiTe_2$. This study is a crucial step for enabling TMTs integration in numerous potential applications in novel micro- and nano-electronics to thermoelectric devices.

Acknowledgements

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Single source precursor pathway towards CVD of MoS_2 thin films

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The recent surge of interest in 2D materials, specifically transition metal dichalcogenides (TMDCs) like MoS_2, is driven by their potential for future technological applications. These applications include implementing TMDCs in thin film transistors (TFTs), photovoltaics, batteries, sensors, and as catalyst materials for the electrocatalytic hydrogen evolution reaction (HER), among others.[1]. However, for scaling up to be implemented in industrial applications, controlled growth of thin TMDC layers is needed on large area substrates, which is quite challenging. Reports on fabrication of 2D-MoS_2 mainly focus on exfoliation or chemical vapor deposition (CVD) methods, which involve sulfurization of molybdenum oxide or using metal halides with H_2S.[2] While exfoliation produces device quality materials, its scalability and thickness control is limited. In contrast, CVD employing molybdenum halides (e.g., $MoCl_5$, MoF_6) with H_2S as a co-reactant[2] is often used for large-area growth of crystalline MoS_2. However, the process involves high deposition temperatures and corrosive by-products that are formed can be harmful.[3] To overcome the drawbacks of the aforementioned precursors, metalorganic precursors of Mo can be utilized in combination with elemental sulfur, enabling film growth under moderate process conditions and avoiding the toxic H_2S.[4] Another promising alternative for further simplifying the processing of MoS_2 film growth involves the use of single source precursors (SSP) containing both Mo and S in one molecule, which was targeted in this study.

We present a new metalorganic chemical vapor deposition (MOCVD) process using a SSP $[Mo(S^tBu)_4]$ (**I**) where the Mo metal is surrounded with a sulfur-coordinated ligand (**Figure 1**). This precursor was reported earlier[5] and in our study, we investigated the role of this precursor on MoS_2 thin film growth, morphology, structure, composition, and optical properties. **Figure 1** illustrates the formation of hexagonal MoS_2 phase in a broad temperature range (450– 700 °C). The phase formation is additionally confirmed by Raman analysis depicted in the figure. The simplified approach to obtain large area, high purity, and stoichiometric thin crystalline MoS_2 layers under moderate process conditions is highly encouraging. This paves the way for further investigation of the films for electrocatalytic and electronic applications.

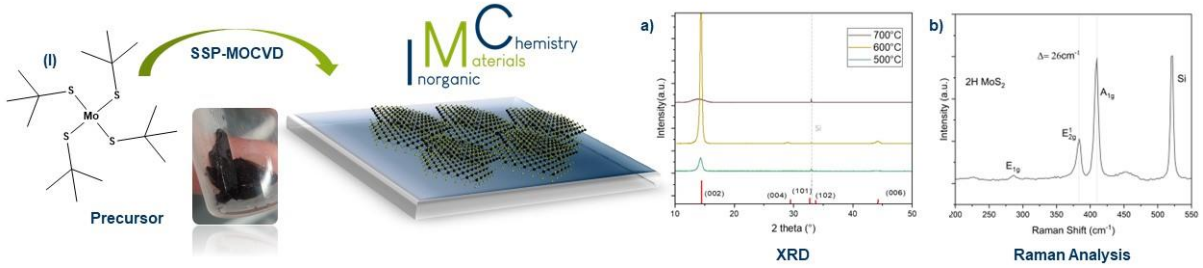

Figure 1. (left) Schematic illustration of the MOCVD process approach for MoS_2, (middle) XRD patterns and (right) Raman analysis of films grown on Si substrates.

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Synthesis of Pristine and Nitrogen-doped Graphene using solid precursors via CVD for SERS application

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Controlled synthesis of large-area high-quality graphene films has become essential for electronic and optoelectronic applications. The chemical vapour deposition (CVD) technique has proven to be at the forefront in bottom-up methods for synthesizing large-area continuous graphene films [1]. Various solid precursors have been used for graphene growth alternative to the gaseous precursor methane [2,3]. In this work, we report the synthesis of graphene and nitrogen-doped graphene (NDG) using solid precursors by evaporating and transporting them onto a copper substrate via atmospheric pressure CVD. Polymethylmethycralate (PMMA) is a carbon-containing polymer utilized for graphene synthesis. The amount of PMMA was optimized as it evaporates and simultaneously gets polymerized, which ceases to evaporate after a certain time, hindering graphene growth. The largest single-crystal graphene obtained is about 180 µm. A large area of continuous graphene film was synthesized after optimizing the growth parameters. The NDG films were synthesized using carbon and nitrogen-containing solid precursor phthalocyanine. As the growth time increases, the graphitic-N configuration has been dominated, and a decrement in N-dopants concentration was observed.

These grown graphene and nitrogen-doped graphene films have been utilized for surface-enhanced Raman spectroscopy (SERS) applications. It was shown that graphene could act as a SERS substrate for sensing the low concentrations of organic dyes [4]. We compared the SERS behaviour of graphene and different configuration of nitrogen-doped graphene. The enhancement factor for pyrrolic-N NDG was found to be 10^5, two orders more than the pristine graphene. Pyrrollic-NDG has shown more enhancement for dyes than graphitic-N NDG.

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Exploring gas phase processed tungsten sulfides for gas sensing applications

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The growing attention towards environmental protection leads to increasing demands on reliable and selective gas sensors to ensure industrial safety and allow environmental monitoring of air pollution and greenhouse gases. Gas sensors based on metal oxide semiconductors have been extensively studied, but their high working temperatures necessitates the search for alternative sensing materials. 2D materials such as transition metal dichalcogenides (TMDC) offer high sensitivity due to large surface area and together with their promising electrical and mechanical properties, render them as a promising material class for the next generation of sensitive and selective gas sensors.[1,2] Application of TMDCs for the gas sensing applications, requires scalable fabrication routes that enable precise thickness control. Bottom-up approaches such as chemical vapor deposition (CVD) routes can meet these demands, but the thin film characteristics strongly depend on the process parameters used including precursors, substrates, deposition temperatures etc.[3]

In our attempts to develop new CVD processes for crystalline TMDC layers, we applied a volatile, reactive, and thermally stable tungsten precursor, namely $[W(N\textit{i}Pr_2)_2(N\textit{t}Bu)_2]$ (**1**)[3] in combination with elemental sulfur that resulted in high quality crystalline hexagonal tungsten disulfide (2H-WS_2) films in the temperature range 600 °C - 800 °C. The deposition time and temperature had a strong impact on the growth of the WS_2 layers. While the initial layer formation at 600 °C was horizontal to the substrate surface, it transformed to vertical growth beyond a few layers (**Figure 1a**). These structural features with high surface area are favored for sensing applications and in this context, we deposited thin WS_2 films on special sensor chips consisting of ceramics with Pt contacts and measured the temperature-dependent sensor response. Representative gases such as NO_2, CO and NH_3 were used as analytes using WS_2 as the sensing material, which revealed a p-type response with varying sensitivities (**Figure 1b**). The results showed encouraging sensitivities towards NO_2 and NH_3 (**Figure 1b**) at temperatures as low as 130 °C. These are very promising developments and is one of the first studies on using CVD derived WS_2 for gas sensing. Moreover, as the operation temperature of the sensor is as low as 130 °C, the implementation of these layers into flexible sensor devices is plausible.

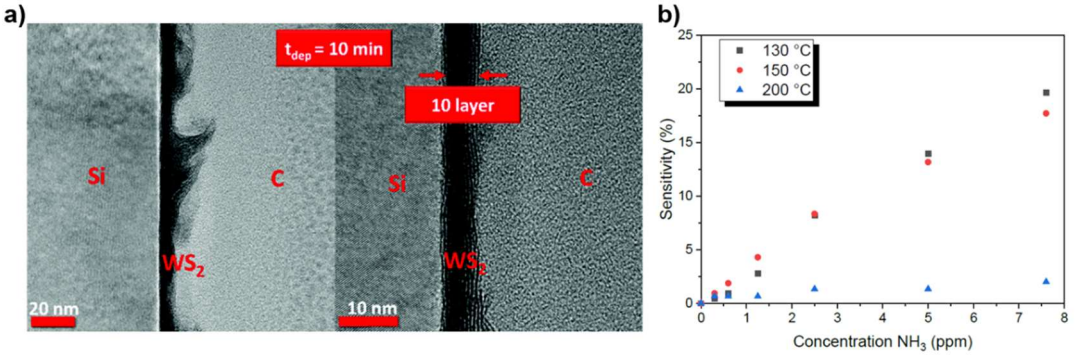

Figure 1. a) Cross-sectional HR-TEM images of 2H-WS_2 films on Si(100). b) Sensitivity of the WS_2 sensor towards NH_3 as a function of heater temperature.[3]

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Layered materials as a platform for quantum technologies

Andrea Ferrari

Layered materials are taking centre stage in the ever-increasing research effort to develop material platforms for quantum technologies. We are at the dawn of the era of layered quantum materials. Their optical, electronic, magnetic, thermal and mechanical properties make them attractive for most aspects of this global pursuit. Layered materials have already shown potential as scalable components, including quantum light sources, photon detectors and nanoscale sensors, and have enabled research of new phases of matter within the broader field of quantum simulations. I will discuss opportunities and challenges faced by layered materials within the landscape of material platforms for quantum technologies, with focus on applications that rely on light–matter interfaces[1].

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Ultra Clean Contacts on Two Dimensional Semiconductors

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*Email: mc209@cam.ac.uk

Exploitation of fundamental properties of atomically thin (two-dimensional, 2D) semiconductors – particularly those from the transition metal dichalcogenide (TMD) family – for electronics will require ultra-clean contacts with resistances approaching the quantum limit. The lack of high quality, low contact resistance p- and n-type contacts on 2D semiconductors has limited progress in next generation of low power devices such as the tunnel field effect transistors. In this presentation, we summarize strategies and provide guidance for making clean van der Waals (vdWs) contacts on mono-layered semiconductors that can efficiently inject both spins and charges.

Contact resistance for Metal-TMD heterostructures: Ab initio study

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Abstract:

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have high mobility, layer-dependent electronic properties, and free from dangling bonds makes them suitable for efficient next-generation semiconducting devices. TMD van der Waals (vdW) heterostructures have strong interlayer coupling over homostructures that leads to better transport properties through emergence of new energy bands with fast carrier dynamics [1–2]. Currently, these advantages are being utilized in many low-power optoelectronic devices including photodetectors, tunnel diodes, transistors, memory devices, etc. [2–5]. However, in practical devices, the charge carrier transport is affected by the high contact resistance because of tunnel barriers as well as Schottky barriers at the interface between electrodes and semiconductors. Hence, we need to identify suitable materials for reducing the barrier heights at metal-semiconductor or semiconductor-semiconductor interfaces to enhance the carrier transport properties. Here, we undertake a systematic investigation on metal-semiconductor and semiconductor-semiconductor interfaces of 2D TMDs. In this presentation, we will show the results of first-principles calculations of the tunnel barrier heights and Schottky barrier heights for the interfaces of different metals and MX_2 (M = metal, X = chalcogen) heterostructures (one of the examples are shown in Figure 1). We have compared these interfacial characteristics for both bottom and top contacts to the TMD heterostructures. By computing the electronic properties of the metal-semiconductor interfaces, we observed that the barrier heights are reduced in case of metal as a top contact with suitable heterostructure. We also present experimental I-V characterization of these metal-TMD heterostructure interfaces and will provide comprehensive comparison with simulations.

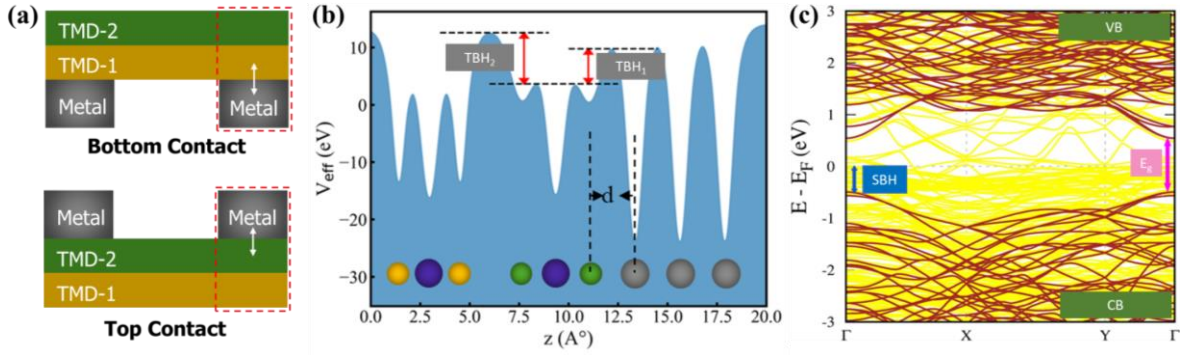

Figure 1. (a) Schematic for bottom & top contact, (b) effective potential plot showing the tunnel barrier and (c) bandstructure showing the Schottky barrier for top contact.

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Multifunctional Memristors Based on Two-Dimensional Layered Materials

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The human brain is the most efficient machine around us in size and power efficiency for self-learning and decision-making capabilities, and simultaneous data storage and processing. Our brain also performs all operations analogously by consuming energy of about 1 – 100 fJ per synaptic event. Even though the conventional computer works much faster than the brain, the von Neumann bottleneck and memory wall issues limit the performance and energy efficiency due to having physically separated storage and processing units. After discovering memristor (MR), a two-terminal device with multiple conducting states at a particular bias voltage, efforts are underway toward developing machines similar to the brain. Despite massive progress in semiconductor technology, it is still challenging to mimic the functionalities of the synapses and neurons, the basic building blocks of our brain, energy efficiently. Hence, enormous efforts are ongoing to explore robust materials and device architecture to develop memristors, which can efficiently generate brain functions. Layered materials like two-dimensional transition-metal dichalcogenides (2D TMDs) and MXenes are attracted high scientific interest due to their rich physical, chemical, electrical, and optical properties.[1-2] Here, I will introduce our recent developments to show robust resistive switching devices of 2D TMDs and MXene thin films that are efficient for logic gate operation, edge computation, and mimicking brain functions.[3]

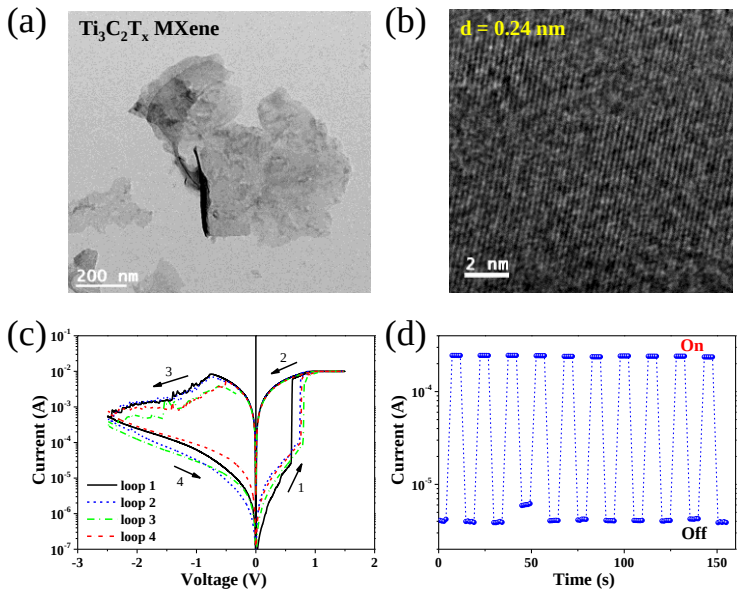

Figure 1. (a & b) TEM and HR-TEM image of $Ti_3C_2T_x$ MXene flake, respectively. (c & d) Current-voltage (*I-V*) characteristics and ReRAM application of MXene thin film, respectively.

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Roles of interactions in layered materials

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Korea Institute for Advanced Study, Seoul, Korea

In this talk, I will discuss critical roles of strong interactions in two-dimensional (2D) crystals and their stacked structures. In 2D crystals, strong interactions between electrons or between electrons and lattices often result in qualitative different electronic, structural and optical properties. Moreover, these materials can be artificially controlled very well such that their thickness or stacking faults can be engineered to demonstrate new physics. So, for each case, a new set of theoretical tools often need to be developed to explain or predict their distinct properties. Novel physical quantities presented in this talk will include preformed charge density wave states, whirlpool phonons as well as weak quasicrystals.

Electrons, excitons and phonons in moiré materials from atomistic simulations

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Beautiful moiré patterns can be created by stacking and twisting two-dimensional crystals, such as graphene or transition metal dichalcogenides. One of the most fascinating discoveries in recent years is that electrons are strongly affected by these moiré patterns and often exhibit completely unexpected behaviour. For example, twisted bilayer graphene – composed of two (semi-)metallic graphene layers – was observed to exhibit correlated insulator states as well as superconductivity at a magic twist angle of 1.1 degrees. In my talk, I will describe my group's efforts to understand the electronic, vibrational and optical properties of moiré materials from an atomistic perspective which is challenging because of the large unit cells in these systems (often containing thousands of atoms). To overcome this difficulty, we use linear-scaling ab initio methods as well as ab initio-derived tight-binding models and effective moiré-scale models. These techniques give detailed insights into the material-specific properties of moiré materials, such as the ordering of K-derived and Gamma-derived valence bands.

Exceptional Points in a Non-Hermitian anisotropic exciton-polariton pair system

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In recent years, microcavity polaritons have emerged as a highly accessible and tunable non-Hermitian system due to their inherently non-conservative nature, offering the potential to realize exceptional points (EPs) and non-trivial topological phases [1,2]. In this work [3], by embedding an optically biaxial semiconductor (few-layer Rhenium disulfide [4]) in an optical microcavity, we obtain two polarized non-orthogonal polariton pairs resulting from the two linearly polarized exciton species in ReS_2 coupling with the degeneracy-lifted transverse electric (TE) and transverse magnetic (TM) cavity modes. The polariton pairs display variable dispersion and coupling strength depending on the polarization state of the probe beam, and the orientation of the sample in the laboratory frame. This tunability facilitates the observation of two classes of EPs in the same system where the polariton branches coalesce. We thus realize a condensed matter system with multiple EPs with the potential to observe non-Hermitian topological invariants and even realize quantum PT-symmetry by introducing a gain mechanism [5], which marks a significant advance in the field of non-Hermitian physics, with potential applications in nano-photonics.

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Engineering of excitonic lineshape and valley dynamics in two dimensional semiconductors using low-cost strain tuning

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Atomically thin two-dimensional semiconductors have received much research interest recently from the photonics community due to their strong light-matter interaction, direct bandgap in the monolayer limit and large exciton binding energy [1, 2]. The integration of these TMDs with the nanostructures is essential for the various applications such as photovoltaic devices, photodetectors and modulators[3, 4, 5]. Being atomically thin, the optical properties of these TMDs have been shown to be easily tunable via application of strain. In particular the exciton binding energy and oscillator strength can be tuned on demand using strain[6]. Strain can be applied either via specialized probe tips used in near field microscopy or by just placing the TMD on top of nanostructures. On the other hand, the emission of TMDs can also be modified by placing them in proximity with metallic nanostructures, which support surface electromagnetic modes called plasmons. These plasmons support extremely large local electric fields and at the same provide high local optical density of states, thereby increasing the exciton emission rate via Purcell effect. These two-dimensional materials also opens promising quantum information technology by using valley pseudospin. The valley polarization can also be tuned by using the strain.

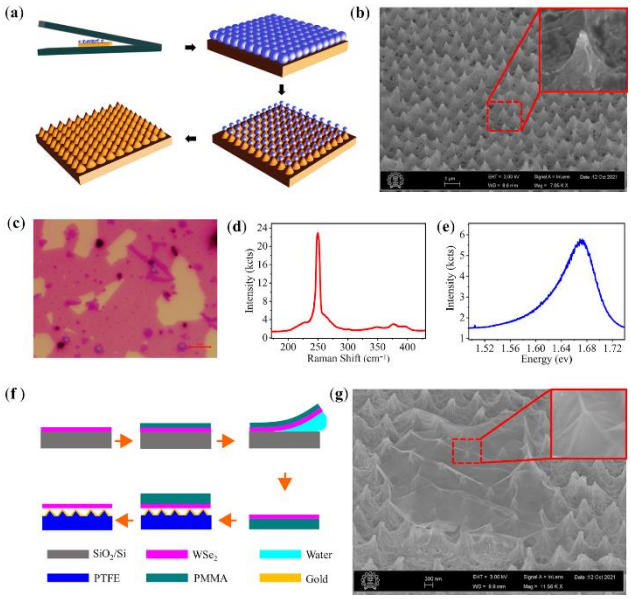

Figure: (a). Schematic of the fabrication of the nanocone, (b). SEM image of the PTFE nanocones (c). CVD grown WSe_2 monolayer (d,e). Raman and PL spectrum of the monolayer WSe_2 (f). Schematic of the Wet transfer method (g). monolayer integrated with the WSe_2

Here we are opening a new low-cost technique to generate the strain in two dimensional materials. By generating strain we tune the line-shape of excitonic emission and simultaneous effect of strain on the valley polarization of the 2D material. We use polystyrene beads as colloidal particles, and a self-assembled monolayer of these particles was deposited via convective self-assembly over a PTFE substrate. The self-assembled monolayer of these colloidal particles works as a mask, which is subsequently etched using reactive ion etching, which causes the formation of the PTFE nanocone array. A thin layer of gold is deposited on top of these nanocone structures, which creates the dual effect of strain and plasmonic enhancement. Finally, we integrate our CVD grown monolayer WSe_2 with these nanocone structures, using a wet transfer method (explained in the figure). We demonstrate strain engineering using photoluminescence and Raman spectroscopy.

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TUESDAY, 21 November, 2023		
Session 4A, GBR, Session Chair: Erik Henriksen		
4A-1	09:00-09:30	**[Keynote] Changgu Lee** Electrical characterization of 2D ferromagnetic materials
4A-2	09:30-10:00	**[Invited] Jorge Vallejo-Bustamante** Singular orbital diamagnetism and paramagnetism in graphene
4A-3	10:00-10:15	**[Contributed] Aparna Parappurath** Band structure sensitive photoresponse in twisted bilayer graphene proximitized with WSe2
4A-4	10:15-10:30	**[Contributed] Sk Md Obaidulla** Room-temperature photoinduced interlayer exciton emission in atomically thin 2D-transition metal dichalcogenide/Organic van der Waals heterostructure
Session 4B, Lalit 1-2, Session Chair: Bent Weber		
4B-1	09:00-09:30	**[Invited] Saptarshi Das** A Graphene-based smart "Electronic Tongue" for highly selective chemi-sensing
4B-2	09:30-10:00	**[Invited] Saurabh Lodha** Few-layer 2D TMD-based photo and strain detectors
4B-3	10:00-10:15	**[Contributed] Pranav** One-step simultaneous liquid phase exfoliation-induced chirality in graphene and their chirality-mediated microRNA delivery
4B-4	10:15-10:30	**[Contributed] Sudarsan Majumder** Ultra-thin chemically derived graphene electrodes for bottom-contacted organic thin-film transistors
Session 4C, Lalit 3-4, Session Chair: Ananth Govind Rajan		
4C-1	09:00-09:30	**[Invited] Amit Kumar Agarwal** Intrinsic Hall and longitudinal non-linear charge transport
4C-2	09:30-10:00	**[Invited] Wang Yao** Layertronics and quantum geometric properties in twisted bilayers
4C-3	10:00-10:15	**[Contributed] Debottam Mandal** Dissipationless intrinsic third-order Hall effect
4C-4	10:15-10:30	**[Contributed] N. Bijoy** Are devices made with twisted bilayers of MoSe2 stable against sliding?
COFFEE BREAK, 10:30-11:00		

Session 5A, GBR, Session Chair: Hridis Pal		
5A-1	11:00-11:30	**[Keynote] Priya Mahadevan** Why do twisted bilayers behave differently from their untwisted counterparts?
5A-2	11:30-12:00	**[Invited] Jeil Jung** Atomistic modeling of single and double moire patterned graphene and hexagonal boron nitride multilayer systems
5A-3	12:00-12:15	**[Contributed] Takaaki V. Joya** Shift current response in twisted double bilayer graphene
5A-4	12:15-12:30	**[Contributed] Swastik Sahoo** Straintronics Using the 2D-Xenes Platform
Session 5B, Lalit 1-2, Session Chair: M.M. Shaijumon		
5B-1	11:00-11:30	**[Invited] Sandhya Susarla** Atomic scale imaging of excitons in twisted two-dimensional materials
5B-2	11:30-12:00	**[Invited] Goki Eda** Upconversion light emission in plasmonic van der Waals tunnel diodes
5B-3	12:00-12:15	**[Contributed] Navaneeth Krishnan K.** Two-Dimensional MoS2 Photodetector: Role of Grain Boundaries and Optic-Nerve Functionality
5B-4	12:15-12:30	**[Contributed] Pawan Kumar** 200 mm Industrial reactor-based monolayer TMDCs growth and defectivity optimization
Session 5C, Lalit 3-4, Focus session on Scientific Publishing, Session Chair: Manish Jain		
5C-1	11:00-11:30	**[Invited] Mayra Castro**, Springer Nature
5C-2	11:30-12:00	**[Invited] Hari Dahal,** Physical Review Materials (APS)
5C-3	12:00-12:30	**[Invited] Thomas Sharp**, IOP Publishing
LUNCH BREAK: 12:30-14:00		
RPGR International Advisory Board (IAB) meeting, Lalit Board Room, 12:30-1.30 PM		
Poster session 2, Exhibition Hall		
P2	14:00-15:30	**Poster Session**
COFFEE BREAK: 15:30-16:00		
Session 6A, GBR, Focus session on Quantum technologies, Session Chair: Manish Chhowalla		

6A-1	16:00-16:30	**[Keynote] Klaus Ensslin** Graphene Quantum devices
6A-2	16:30-17:00	**[Invited] Bent Weber** Towards quantum electronics and optoelectronics with individual point defects in 2D semiconductors
6A-3	17:00-17:30	**[Invited] Chandan Kumar** Harnessing 2D Van der Waals Materials for Quantum Sensing Technology
Session 6B, Lalit 1-2, Session Chair: Jeil Jung		
6B-1	16:00-16:30	**[Invited] Debjani Karmakar** Spin-dynamical magnetism in 2D-Kagome plane of Superconducting AV3Sb5 (A = Cs, Rb, K)
6B-2	16:30-17:00	**[Invited] Madhav Prasad Ghimire** Pressure induced evolution of Fermi surface and de Haas-van Alphen effect in CsV3Sb5
6B-3	17:00-17:15	**[Contributed] Sayan Kanungo** Asymmetric Interlayer Chalcogen Pairing Induced Type 2 Band Alignment and Energy Bandgap Reduction in Two Dimensional Bilayer Janus SnSSe
6B-4	17:15-17:30	**[Contributed] Kanchan Ulman** Excitons and Exciton-Phonon Coupling in Organic-2D material Heterostructures
Session 6C, Lalit 3-4, Session Chair: TBC		
6C-1	16:00-16:30	**[Invited] Ritesh Agarwal** 3D Twistronic Photogalvanic Effect - A New Paradigm of Light-Matter Interaction in a Twisted Coordinate Frame
6C-2	16:30-17:00	**[Invited] U. Chandni** Spin-orbit coupling enhanced valley ordering and orbital magnetism in twisted bilayer graphene
6C-3	17:00-17:15	**[Contributed] Albert F. Rigosi** Using Graphene and 2D Topological Insulators as a Global Standard for Quantum Electrical Units
6C-4	17:15-17:30	**[Contributed] Atindra Nath Pal** Detection of nontrivial topology driven by charge density wave in a layered semi-Dirac metal
YOUNG RESEARCHERS' MEET UP AND NETWORKING SESSION, GBR		
YRM	17:30-18:00	**Panelists: Vidya Kochat (IIT Kharagpur), Ashish Arora (IISER Pune), Ananth Govind Rajan (IISc Bangalore)**

Electrical characterization of 2D ferromagnetic materials

The representative 2D materials, graphene, h-BN, and MoS2, have interesting mechanical, electrical and optical properties and have exhibited fascinating physical phenomena so far. However, they mostly lack one important physical property in physics, magnetism. The new 2D materials such as CrSiTe3, CrI3, and FePS3, which began to be studied recently, possess ferro-(FM) or antiferro-magentic(AFM) properties even in atomic level thickness and are expected to reveal deep level of physics in 2-dimensional confinement.

In this presentation, we will discuss our recent research on the magnetic properties of ternary 2D materials, specifically Fe3GeTe2 and Fe5GeTe2. These materials exhibit ferromagnetic behavior and possess relatively high Curie temperatures. We conducted hall measurements to study their magnetic characteristics. The hall measurement results revealed that Fe3GeTe2 displays the anomalous hall effect due to its intrinsic ferromagnetism. Moreover, we observed significant changes in magnetic properties, such as coercivity, as the thickness of Fe3GeTe2 decreased, transitioning from weak ferromagnetism to strong ferromagnetism. Furthermore, when Fe3GeTe2 was stacked with 2D antiferromagnetic materials, we observed the occurrence of exchange bias. Notably, this phenomenon was only observed when both the FM and AFM materials exhibited the same type of magnetic order, and not for different types. Since the AFM materials used in our experiments were semiconductors, we were able to observe variations in magnetic properties dependent on the applied gate voltage. Moving on to Fe5GeTe2-based electric devices, we found that the application of an electric bias resulted in a current-dependent phase change between FM and AFM states. Numerical calculations suggest that this phase change arises from modifications in the RKKY interaction between the layers, influenced by the nonhomogeneous potential distribution within the device.

In summary, our research sheds light on the magnetic properties of Fe3GeTe2 and Fe5GeTe2 in the context of 2D materials, highlighting their ferromagnetic behavior, thickness-dependent changes, and interactions with AFM materials and electric bias.

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Singular orbital diamagnetism and paramagnetism in graphene

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Graphene is one the most studied materials in condensed matter because of its astonishing properties related to its linear dispersion relation. One of these properties is the diamagnetic divergent orbital susceptibility at the Dirac point. This characteristic, which is a striking signature of the anomalous π Berry phase in graphene, was predicted many decades before, but it has been challenging to measure at a single-flake level. Another exciting prediction concerns the orbital magnetism of 2D crystals in general. The existence of a divergent orbital paramagnetic susceptibility has been predicted. These singularities are expected at the saddle points of the band structure.

To realize our experiments, we have used a new technique that involves highly sensitive giant magneto-resistant (GMR) probes in combination with chemical potential control through a gate modulation. By the means of this technique, we have measured the singular orbital diamagnetic susceptibility in monolayer graphene, for the first time at single-flake level [1]. We have also measured the singular orbital paramagnetic susceptibility in graphene in a moiré superpotential that comes from the alignment of graphene and boron nitride [2].

Our results open a new way to explore the orbital magnetism and currents in 2D materials. This experiment should also complement the investigation of the particularities of the geometry of the band structure of 2D crystals, particularly Berry phase anomalies or saddle points, or reveal the existence of ballistic loop currents along the edges of 2D topological insulators.

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Band structure sensitive photoresponse in twisted bilayer graphene proximitized with WSe_2

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The ability to tune the twist angle between different layers of two-dimensional (2D) materials has enabled the creation of flat bands artificially, leading to exotic quantum phases. An emerging direction in this field is twisted bilayer graphene (tBLG) van der Waals coupled to a layer of semiconducting transition metal dichalcogenide, such as WSe_2, which leads to unique electronic and structural properties arising from moir´e superlattice potential, proximity-induced spin-orbit interaction, etc. Although different transport measurements have shed light on the rich-phase diagram of WSe_2/tBLG devices, understanding light-matter interaction in such systems remains elusive. Here we have leveraged WSe_2/tBLG heterostructure to perform photoresponse measurements, where the mis-orientation angle of the tBLG layer was chosen to lie close to the magic angle of 1.1^o. Our experiments show that the photoresponse is extremely sensitive to the band structure of tBLG. We demonstrate that photogating emerges as a primary mechanism for photoresponse in the tBLG layer prevailing above the moir´e band edge. In contrast, strong suppression of photoresponse is observed as the Fermi level is tuned inside moir´e flat bands at low temperatures. Our observations suggest that the screening effects from moir´e flat bands strongly affect the charge transfer process at the WSe_2/tBLG interface, which is further supported by time-resolved photo-resistance measurements. With the enhanced photo responsivity arising from the photogating effect, our device architecture opens up new possibilities to optoelectronically probe the rich physics of WSe_2 proximitized tBLG.

Room-temperature photoinduced interlayer exciton emission in atomically thin 2D-transition metal dichalcogenide/Organic van der Waals heterostructure

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Hybrid heterostructures comprising atomically thin two-dimensional transition metal dichalcogenides (2D-TMDs) and molecule could modulate the optoelectronic and transport properties outstandingly.[1] The interlayer excitons (ILX) or spatially indirect excitons (1–1.3 eV) are electrons and holes that are bound by Coulomb interactions but spatially separated in two different layers. While in a 2D/2D system, spatially indirect excitons in heterostructures have been extensively explored.[2] The reduced oscillator strength and room-temperature instability typically renders them dark and hard to access for future applications.[3]

Here, we demonstrate a room temperature stable novel ILX emission peak with relatively large oscillator strength at around 2.18 eV in a CVD synthesized 2D MoS_2 monolayer covered by few nm thick (5 nm) organic molecule (metal phthalocyanine, MPc), forming a 'type-II' p-n junction-based heterostructure (Figure1). Additionally, we discuss this newly-emerging TMDO heterostructures, including their synthesis methods and transport behavior of field-effect devices. By engineering 'type-II' band gap alignment in a TMDO heterostructure, we show the current mechanism of enhanced oscillator strength and significant advancement of ILX emission and its modulation. Therefore, 2D TMD materials and organic semiconductors offer a unique platform for addressing many underlying physics, such as electrically tunable static dipole with long-range (long life-time ~100 ns - 1μs) dipole interactions, promising rich many-body quantum phenomena—strong exciton correlations, enhanced temporal coherence time, or the formation of relatively high temperature Bose–Einstein condensation.[4]

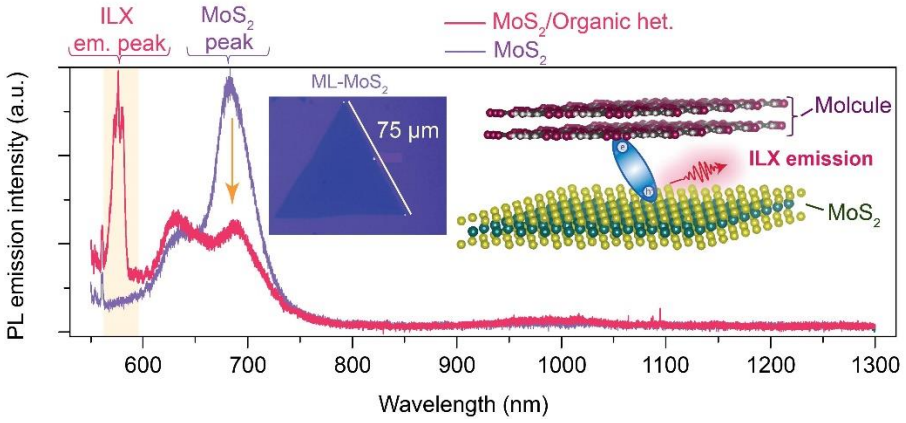

Figure 1. PL of MoS_2/MPc heterostructure. ILX emission peaks appears at 570 nm (~2.18 eV).

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A Graphene-based Electronic Tongue

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In this abstract, we present a novel interdisciplinary approach that integrates the computational power of machine learning with the unique chemisensing properties of graphene to engineer an "electronic tongue." This state-of-the-art device leverages the sensitivity and specificity of graphene-based sensors to detect minute chemical changes, while machine learning algorithms process and interpret complex data patterns. The primary objective is threefold: to ascertain food authenticity, detect molecular markers of adulteration, and identify early-stage chemical indicators of spoilage. This synthesis of advanced materials and computational methodologies offers a paradigm shift in the field of food quality assessment, paving the way for more rigorous, real-time evaluations of food integrity and safety.

Few-layer 2D TMD-based photo and strain detectors

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In recent years, researchers have leveraged the unique physical properties of layered two-dimensional (2D) van der Waals (vdW) materials, such as a wide range of thickness-tunable bandgaps, excellent light-matter interaction and facile fabrication of heterostructures with defect-free heterointerfaces, for several optoelectronic applications. At the same time, their ultra-thin nature and high tensile strength enables the tuning of bandstructure parameters, and hence their optical and electronic properties, using strain. This presentation will describe recent results from our group on engineering the photo- and strain-detection performance of transistors based on 2D vdW transition metal dichalcogenide (TMD) semiconductors and their heterostructures.

Photoresponsivity and speed of few-layer TMD photodetectors are fundamentally traded-off with each other by modulation of the effective trap concentration, as shown through electrostatically gated supported and suspended ReS_2 photodetectors.[1] This trade-off can be attenuated by nearly 2× using an electrostatically tunable in-plane p-n homojunction integrated laterally with a WSe_2 phototransistor, enabling enhanced photoresponsivity (>100 A/W), and high detectivity (>10^{12} Jones) along with switching speed in the μs range at the same time.[2] Beyond single-TMD photodetection, TMD/TMD heterostructures offer the possibilities of interlayer interface engineering for improving photodetection parameters. For instance, engineering the band alignment from type-II to type-III in a $WSe_2/SnSe_2$ p-n heterodiode helps realize a high negative responsivity of 2 × 10^4 A/W with a fast response time of ~1 μs due to a tunneling photocurrent.[3] Finally, an electrically actuated piezo-stack is shown to fine-tune optical and electrical parameters of MoS_2 field-effect transistors with tensile as well as compressive strain, offering improved control and integration possibilities over existing mechanical methods.[4]

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Research/Clinical Abstract

One-step simultaneous liquid phase exfoliation-induced chirality in graphene and their chirality-mediated microRNA delivery

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Background: Graphene (G) has been established as an exciting prospect for a broad range of applications owing to its remarkable properties. As the molecular structure of G itself is achiral thus introducing chirality in G by simple attachment of a functional group (a chiral ligand) on the G nanosheet may result in more diverse applications. The recent innovations of G chiral nanosystems have been extended to drug delivery. Herein, we have developed a novel and facile synthesis method for producing chiral G for its application in the chirality-dependent microRNA delivery.

Methods: L-graphene and D-graphene were produced in a single step by using chiral L-tyrosine and D-tyrosine as a stabilizing and chiral-inducing agent and applying high-temperature sonication. The chirality of the exfoliated L-graphene and D-graphene was assessed with circular dichroism (CD) spectroscopy and their structural, morphological, and surface evaluations were studied using Raman spectroscopy, transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS), respectively. In addition, an attempt has been made to explore the cell viability, hemocompatibility, cellular uptake, and internalization pathway, chirality-mediated interaction, and microRNA (hsa-miR-205-5p) transfection with C4-2B prostate cancer cells.

Results: The CD spectra confirmed the chirality present in the exfoliated L(D)-Graphene. Moreover, the Raman spectrum and TEM data confirmed the formation of multi-layer graphene with asymmetric morphology and a large aspect ratio. L-graphene and D-graphene show cellular compatibility. Chiral preferential binding occurring between miR-205 and D-graphene makes them an exciting prospect for gene delivery. D-graphene exhibits superior hemocompatibility compared to commercially available transfection reagent (Lipofectamine). Cellular uptake is clearly shown by internalization of D-graphene into C4-2B prostate cancer cells. miR-205 efficient delivery utilizing D-graphene was confirmed by transfection efficiency and MTT assay.

Conclusions: Our results demonstrated that a direct approach- one-step liquid phase exfoliation-induced chirality in graphene and their selective chirality-mediated microRNA delivery.

Ultra-thin chemically derived graphene electrodes for bottom-contacted organic thin-film transistors

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Abstract: Graphene has shown promise as an extremely efficient electrode material owing to its high chemical stability, superlative mechanical strength, good optical transparency, high carrier mobility and suitable work function[1]. However, relevant low-cost graphene synthesis techniques for research applications like mechanical exfoliation fail to deliver as a potential electrode manufacturing route due to challenges in mass fabrication. Although wafer-scale CVD graphene synthesis offers a possible solution to batch processing, it entails a high thermal budget, greater time complexity and increased cost of production. With the consideration that bottom contact configuration is the most commonly used architecture for organic field effect transistors[2], solution processing of graphene oxide and subsequent reduction to chemically derived graphene (CDG), also known as reduced graphene oxide (rGO), offers a facile route to fabricating bottom electrodes for contacting organic field effect transistors (OTFTs) with reduced cost and availability in abundance[3,4]. This work shows that using photolithographically patterned ultra-thin (~ 4 nm) CDG electrodes, solution-processed OTFTs can be fabricated and characterised with very low to negligible contact effect. In our experiments, Poly[2,5-bis(3-dodecylthiophen-2-yl)thieno[3,2-b]thiophene], commonly known as PBTTT, was used as the organic material for the fabricated OTFTs. In our measurements, the current-voltage characteristics show a very good quadratic transition into the saturation from the linear region with negligible contact resistance, even at low drain-source voltages. Compared to the previous reports[4], we propose that the use of extremely thin CDG electrodes offers a better interface morphology and contact with the organic material, leading to superior performance.

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Intrinsic Hall and longitudinal non-linear charge transport

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Band geometric properties of Bloch electrons give rise to several interesting optical and transport phenomena in quantum systems. Examples include the Berry curvature induced anomalous Hall effect, and the Berry curvature dipole and quantum metric dipole induced nonlinear Hall effects. Here, we predict a new intrinsic and dissipationless third-order Hall responses in systems that break time-reversal symmetry. We systematically derive the general expression of third-order conductivities, both intrinsic and extrinsic, and show that these exciting third-order Hall responses arise from the band geometric quantities such as Berry curvature, quantum metric, geometric connection, and the second-order connection. We demonstrate our results for the magnetically gapped surface states of spin-polarised electrons, realised by two-dimensional massive Dirac Hamiltonians. These novel third-order Hall effects offer a new way to probe band topologies, and open new avenues for potential electronic and optoelectronic applications.

Layertronics and quantum geometric properties in twisted bilayers

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Twisted stacking and formation of moire superlattices have provided powerful approach towards designer quantum materials. In this talk, I will focus on the quantum geometric properties of electrons in twisted homobilayers of TMDs and graphene, arising from the layer quantum degree of freedom when twisting introduces layer pseudospin texture in real space and in momentum space. Small angle twisted R-stacking TMDs hosts a honeycomb moire with the two triangular sublattices residing on opposite layers, and real-space Berry phase from such a layer pseudospin texture realizes an emergent magnetic field [1,2], underlying the Kane-Mele type topological dispersion in lowest minibands. Combined with intrinsic ferromagnetism from the direct Coulomb exchange between moire orbitals [3], such a layer-sublattice locked moire superlattice has become an exciting platform for exploring quantum anomalous Hall effect. Besides the gate tunable ferromagnetic QAH observed in twisted $MoTe_2$ [4], our Hartree Fock calculation also reveals the existence of an altermagnetic orbital Chern insulator at filling factor 2, where the sizable orbital magnetization makes possible initialization of the spin Neel order and the Chern number in applied magnetic field, and Chern number can be electrically switched sign at zero magnetic field [5]. I will also discuss novel Hall effects of various band geometric origin in twisted homobilayers over broad range of twisting angles, including the time-reversal even linear Hall counter flow [6], and the nonlinear dynamical Hall effect of a crossed geometry [7].

The work was supported by Research Grant Council of HKSAR (AoE/P-701/20, HKU SRFS2122-7S05), Croucher Foundation, and the New Cornerstone Science Foundation.

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Dissipationless intrinsic third-order Hall effect

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The Band geometric properties of Bloch electrons play a crucial role in many interesting optical and transport phenomena in quantum systems. Examples include the Berry curvature induced anomalous Hall effect and the dipole of Berry curvature or quantum metric induced nonlinear Hall effect. Here, we predict new intrinsic and dissipationless third-order Hall responses in systems that break time-reversal symmetry. We systematically derive the general expression of third-order conductivities, both intrinsic and extrinsic, using the quantum kinetic theory in conjugation with the relaxation time approximation. These exciting third-order Hall responses arise from the band geometric quantities such as Berry curvature, quantum metric, geometric connection, and the second order connection. We demonstrate our results for the magnetically gapped surface states of spin-polarised electrons, realised by two-dimensional massive Dirac Hamiltonians. These novel third-order Hall effects offer a new way to probe higher rank band geometric quantities and can be used for potential electronic and optoelectronic applications.

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Are devices made with twisted bilayers of $MoSe_2$ stable against sliding?

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Mo and W based transition metal dichalcogenides have been best known as semiconductors and solid state lubricants, the latter emerging from the weak van der Waals bonding existing between different layers in these materials. There has been recent interest in constructing heterostructures out of them by peeling off layer by layer in a controlled manner and building a stack with two or more layers. The heterostructures built in this manner are different from the naturally occurring bulk structures of these materials that have a particular registry associated with them. However, this approach gives one the additional freedom of being able to rotate one layer with respect to another, leading to commensurate unit cells in some instances, depending on the angle of rotation. A motorised approach allows enormous control of almost 0.2 degree while constructing these heterostructures, and various devices have been made with properties very different from the unrotated limit [1, 2]. However, the question we explore here are examining the changes in the electronic structure if in addition to the twist, one additionally has an unintentional displacement of the top layer in twisted bilayers. Is one still looking at the same device?

We start by considering a large angle of twist, far away from the small twist angle region where interesting phenomena have been seen. The atomic positions in the constructed structure have been optimised. We then allow for displacements in various directions away from this point and explore the ensuing changes in the structure as well as the electronic structure. A similar exercise is carried out for small angles of rotation, and the implications of these results will be discussed.

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Why do twisted bilayers behave differently from their untwisted counterparts?

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The Mo and W based transition metal dichalcogenides have been known for several decades as examples of semiconductors whose electronic structure is well described by band theory. It is only recently that one finds unusual phenomena arising in them on doping holes via gating into twisted bilayers [1], an aspect that we would associate with correlated materials. We have recently examined the electronic structure of twisted bilayers of Mo [2] and W [3] based transition metal dichalcogenides. In contrast to graphene, we find the emergence of flat bands for several angles of rotation. The origin of this can be linked to patches of various types of stackings which include an atom-on-atom as well as a staggered stacking. The former lead to larger inter layer separations because of the larger repulsion between the electrons in the two layers in contrast to the latter. This leads to larger perturbations in some regions of the moire cell. Building on the fact that these materials represent van der Waals structures, and so the perturbation induced by one layer on the other should be small, we explore different twist angles and quantify the perturbation in each instance from the untwisted limit. Surprisingly, at large twist angles we find that we recover the low energy electronic structure of the untwisted limit, while at small angles we find flat band formation as well as other unusual aspects of the electronic structure.

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Atomistic modeling of single and double moire patterned graphene and hexagonal boron nitride multilayer systems

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The physics of moire materials has emerged as an attractive research topic in condensed matter physics thanks to the possibility of tailoring narrow bandwidth topological band systems prone to strong correlations. In this talk we present efforts from our research group to develop the theoretical and computational framework to improve the predictive accuracy of twisted and untwisted rhombohedral multilayer graphene interfaced with hexagonal boron nitride as prototypical examples where one can generate precursor states leading to orbital magnetism observed in experiments. We discuss the sensitive role of alignment and sliding geometries and relaxation effects in the resulting electronic structure in a few representative moire multilayer systems.

Shift current response in twisted double bilayer graphene

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We present our numerical results on the shift current response in AB-AB and AB-BA stacked twisted double bilayer graphene (TDBG).

The shift current is a second-order nonlinear optical (NLO) response which is accompanied by a real optical transition. Its striking feature is that the output current is dc despite the fact that the input electric field is ac. The shift current is characterised by a quantity known as the shift vector, which is expressed in terms of the difference between the Berry connections of the initial and final band of the optical transition [1]. Due to its relation to the Berry connection, the shift current response is utilised to probe the topology of various materials [2]. Yet, as a downside, NLO responses tend to generate small contributions, which make experimental measurements of these signals a challenge.

Moiré materials is a desirable platform to study NLO responses as they can have a large joint density of states, due to the formation of flat bands, which enhances the NLO response. TDBG is an example of a moiré system that can be prepared by stacking two sheets of untwisted AB stacked bilayer graphene and introducing a relative twist angle. It is known that the two variants of TBDG (AB-AB and AB-BA stacked TDBG) have similar band structures, yet, contrasting valley Chern numbers [3].

In the present study, we are motivated to investigate the effect of the contrasting topology of AB-AB and AB-BA stacked TDBG on the shift current response. Using the effective continuum Hamiltonian for TDBG [3] and through numerical analysis, we have shown that the difference in the topology between the two variants of TDBG manifests as the relative sign of the signal, as shown in Fig. 1. We further show that topological transitions are detectable through the sign flip of the shift current.

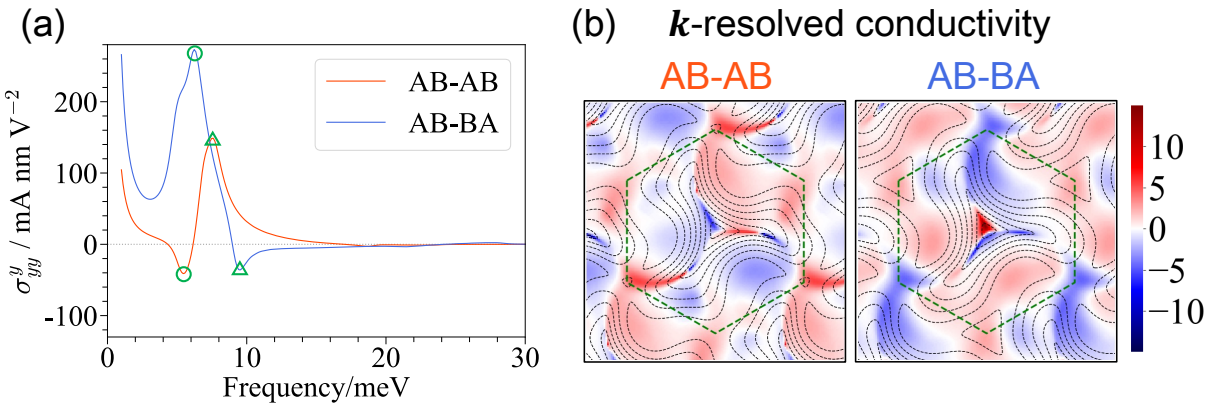

Figure 1. (a) The shift current conductivity of AB-AB and AB-BA TDBG. (b) The *k*-resolved shift current conductivity, given by the colour map, and the energy gap, given by the contour lines.

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Straintronics Using the 2D-Xenes Platform

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The tremendous success of graphene has initiated a paradigm shift towards the expedition of various properties of graphene-like 2-D materials, commonly referred toas Xenes. Silicene is the front runner among the other options, such as germanene, stanene, and phosphorene, to name a few, due to its compatibility with the current silicon fabrication technology. The rapid miniaturization of silicon devices and the beneficial electro-mechanical properties of silicene in the field of flexible electronics [1] have paved the way for the other buckled and puckered xenes mentioned above in nano electro-mechanical systems (NEMS). Based on the results obtained for silicene [2], we propose a model applicable to investigate straintronics in the nanoscale regime for the xenes using ab-initio density functional theory and quantum transport theory approach based on Landauer formalism. The directional piezoresistances have been calculated for the xenes according to their critical strain limit and the gauge factors are compared, which are sinusoidally dependent on the transport angle akin to graphene [3]. Other applications of straintronics have been explored, namely conductance modulation and pressure sensitivity, to mention a few. The former is quantized in nature and exhibits opposite behavior against strain with regards to the critical transport angle, and the latter shows the essential dependence of critical pressure on strain. Based on the above results, we propose a review model for the monolayer xenes keeping the perspective of flexible electronics and their applications.

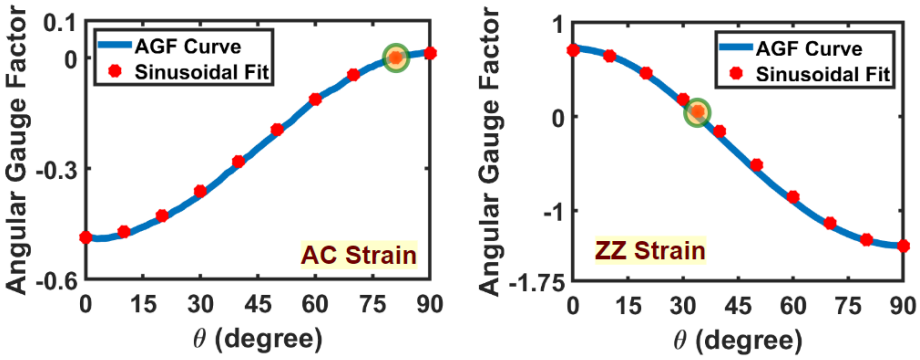

Figure 1. Variation of Gauge factor and it's sinusoidal fit for silicene against transport angle.

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Atomic scale imaging of subtle electronic states in twisted transition metal dichalcogenides

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After the discovery of superconductivity in magic angle bilayer graphene, there is tremendous interest to explore the entangled electronic states in 2D materials due to moiré structures. In transition metal dichalcogenides (TMDs), the inter-layer and intra-layer excitons are often coupled with the moiré potential to form entangled electronic states. Usually, moiré excitons are probed by far-field optical or near-field scanning probe spectroscopies. However, these techniques offer either limited spatial or spectral information. On the other hand, by using low-loss electron energy loss spectroscopy (EELS) we can probe the moiré excitons without compromising the spatial resolution. In my talk, I will elaborate on our group's progress to image excitons from barely detecting them to imaging at the atomic scale using WS_2/WSe_2 heterostructures as the model system. At the end of my talk, I will ponder on some of the future challenges involved in electron spectroscopy and pathways to solve this problem.

I acknowledge the support from ASU FSE startup funds. The electron microscopy work was carried out at the Molecular Foundry at Lawrence Berkeley National Laboratory, Center for Nanophase Materials Sciences at Oak Ridge National Laboratory and Erying Materials Center at Arizona State University. The work at Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02- 05CH1123. STEM research was conducted as part of a user project at the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory. We acknowledge the use of facilities within the Eyring Materials Center at Arizona State University supported in part by NNCI-ECCS-1542160.

Upconversion light emission in plasmonic van der Waals tunnel diodes

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Plasmonic tunnel junctions comprising van der Waals semiconductor are an attractive platform where the interplay between inelastically tunneling electrons, surface plasmons, and excitons is expected to give rise to novel light emission phenomena. Here, we report observation of peculiar upconversion electroluminescene in van der Waals tunnel diodes comprising a monolayer transition metal dichalcogenide (TMD) in the electron tunneling pathway [1]. The device exhibits bimodal electroluminescence with a broad low energy band and a narrow high energy band. Interestingly, the high energy emission, which is attributed to the TMD ground exciton, is found to turn on at applied biases significantly lower than the threshold defined by its emission energy whereas the low energy emission, which arises from plasmonic emission, strictly obeys the quantum cut-off. We examine several possible models and show that momentum-indirect excitation of high energy carriers enabled by inelastic electron tunneling is a key component enabling the apparent energy gain.

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Two-Dimensional MoS_2 Photodetector: Role of Grain Boundaries and Optic-Nerve Functionality

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ABSTRACT

Recent optical imaging systems have restricted power and area efficiency due to the significant peripheral electronics needed for precise imaging. Using an optoelectronic neuromorphic device with short-term plasticity (STP), which is inspired by the visual processing in the retina, the visual system can self-adjust in real time in response to external stimuli, such as light-controlled short-term facilitation (STF) and long-term facilitation (LTF). Here, we investigated MoS_2 shape evolution by controlled chemical vapor deposition and developed optical synaptic devices across the grain boundaries. [1] The effect of grain boundaries is evidenced by demonstrating an optoelectronic synaptic device based on a simple Au/MoS_2/Au lateral structure exhibits synaptic STF, LTF and PPF. STF results from a rise in photocurrent caused by the trap filling by the electrical stimulation previously. [2] Additionally, the device we used shown the famous conditioning experiment like Pavlov's dog. The implementation of self-adjustment through STP in the evolving optoelectronic neuromorphic device may pave the way for bionic devices with different environments.

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200 mm Industrial reactor-based monolayer TMDCs growth and defectivity optimization

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The role of transition metal di-chalcogenides (TMDCs) layers as an advanced logic channel material is shaping rapidly in the research world. The ability of two-dimensional (2D) TMDCs to outperform Si channels on scaled devices makes them an attractive alternative candidate.

Integrating an atomic-thin monolayer at 200 mm wafers is quite challenging at different processing stages. We are narrowing it down by using the growth of 2D layers with two-parallel approaches; Epitaxy and Amorphous layer-supported growth.

Our epitaxial growth on sapphire, involved in the transfer-based route, is advancing towards growing single crystalline monolayer over a 200 mm scale in addition to the formation of twin boundaries.

Reducing grain boundaries is one of the important aspects to reduce overall defectivity. We involve TEM diffraction analyses stitched over large field of view to probe the extension of the crystal domains. The other source of defectivity is mostly related to the presence of intra-grain defects. We are implying the low-temperature photoluminescence and in-situ electrostatic gating techniques to identify the level/character of defectivity at each various of the device integration process.

Following this methodology, we have analyzed different 2D monolayers grown by MOCVD in adapted industrial reactors with different process conditions as well as into lab-based tool (with metal oxide CVD). An effective role of defects being analyzed by these techniques provides us with developing a platform for the industrial integration processes.

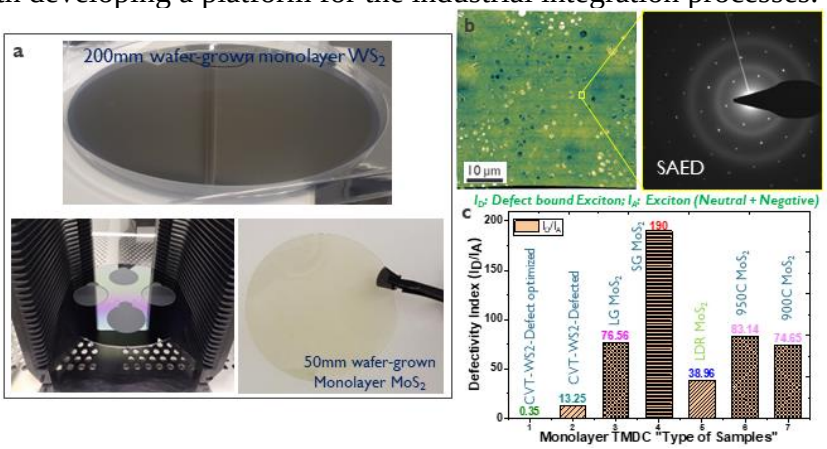

Figure 1. (a) Industrial reactor based 200mm wafer-grown uniform monolayer WS_2 along with pocket-wafer 50mm (2") grown MoS_2 shown using camera-clicked pictures. (b) DigitalMontage stitched false-coloured Dark-field TEM image of monolayer MoS_2 and corresponding SAED pattern presenting the single crystalline nature over the ultra-large area. (c) Defectivity indexation is plotted for the number of monolayers grown in different conditions and analyzed using low-temperature Photoluminescence spectroscopy.

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Graphene Quantum Devices

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This work was done in collaboration with Lisa Maria Gächter, Rebekka Garreis, Chuyao Tong, Max Josef Ruckriegel, Folkert Kornelis de Vries, Annika Kurzmann, Wister Wei Huang, Jonas Gerber, Lara Ostertag, Elías Portolés, Shuichi Iwakiri, Giulia Zheng, Peter Rickhaus, Alexandra Mestre Tora and Thomas Ihn.

ABSTRACT

Quantum dots have emerged as one of the contenders for a future quantum information processor. Bilayer graphene is now established as a material that allows high quality bi-polar Coulomb blockade measurement, time-dependent transport measurements and first relaxation time measurements. In contrast to the more conventional GaAs and Si-based systems, several exiting and unexpected observations in graphene have been explained by the peculiar graphene bandstructure, which is gate-tunable, the additional valley degree of freedom, and spin-valley coupling. Here we demonstrate shell filling of electronic states in graphene quantum dots and derive the spin and valley Hund rules for the first 24 carriers occupying the quantum dots. Lifetimes of single single spins are measured using the Elzermann read-out. For two carriers occupying a single or double quantum dot we find a complex charge stability diagram with transitions governed by Pauli spin and/or valley blockade. Using these two carrier states we measure spin lifetimes of about 50 ms and valley lifetimes approaching 1s. We also present measurement on quantum devices realized in magic-angle-twisted-bilayer-graphene, based on the nature of superconducting states.

Towards quantum electronics and optoelectronics with individual point defects in 2D semiconductors

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Individual point defects and colour centres have become key elements in rapidly maturing quantum technologies, with applications in quantum sensing, computation, simulation, and communication. Different from conventional 3D semiconductors, spins in atomically-thin (2D) semiconductors with hexagonal lattices [1], are coupled to an additional valley degree of freedom [2] in the presence of inversion asymmetry and strong spin-orbit coupling. In-gap states due to atomic point defects can inherit these properties [3], promising coherent control of spin-valley states both electrically and optically. Using low-temperature (4.5K) resonant tunnelling scanning probe spectroscopy, we show that sulphur (S) vacancies in monolayers of MoS_2 exhibit a rich in-gap electronic structure, governed by an interplay of local crystal symmetry breaking and spin-orbit coupling. Further combining the unrivalled spatial resolution of the scanning tunnelling microscope (STM) with conventional optics, we capture electrically stimulated luminescence with single-photon character at length scales two orders of magnitude below the diffraction limit of conventional optics.

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Harnessing 2D Van der Waals Materials for Quantum Sensing Technology

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Recent advancements in the fabrication of high-quality crystals and van der Waals heterostructures have opened new frontiers in the realm of condensed matter physics and quantum sensing technology. This progress has paved the way for the creation of ultra-clean van der Waals heterostructures, providing a versatile platform for emulating the properties of 3D crystals in a 2D setting. This talk explores the remarkable potential of van der Waals materials in the context of quantum sensing and sensor technology.

Van der Waals materials, characterized by their two-dimensional nature, exhibit a broad spectrum of properties, including those of semiconductors, insulators, superconductors, topological insulators, and Weyl semi-metals. These properties are highly dependent on the layering of these materials, enabling them to be stacked in various orders, leading to emergent phenomena not observed in isolated layers.

One of the most intriguing features of van der Waals materials is their exceptional sensitivity to environmental factors such as temperature, magnetic fields, and mechanical strain. Leveraging these properties, they offer an exceptional opportunity to develop compact, low-noise, and ultra-sensitive quantum sensors, with applications spanning across diverse fields, from medical science to materials research and beyond.

In this presentation, we will delve into the immense potential presented by 2D van der Waals materials in the realm of sensor technology. We will explore two specific examples of sensor devices: the single electron transistor and the superconducting quantum interference device. Through these examples, we will highlight the transformative capabilities of van der Waals materials in enabling the development of state-of-the-art quantum sensors, poised to revolutionize a multitude of applications in science and technology.

Spin-dynamical magnetism in 2D-Kagome plane of Superconducting AV3Sb5 (A = Cs, Rb, K)

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The 2D-V-kagome plane of the superconducting series AV_3Sb_5 (A = Cs, Rb and K) hosts an intricate interplay of strong-correlations, non-trivial electronic topology and intriguing fermiology and thus renders the series to be a playground of many mutually dependent exotic phases like charge-order or superconductivity. However, for this system, the interconnection of magnetism and complex collective phenomena and their combined impact on the underlying exotic phases has yet not arrived to any conclusion. Using first-principles based DFT+DMFT analysis; we demonstrate that electron correlations and non-trivial magnetism in conjunction with the spin-orbit coupling have strong influences on their electronic structure, complex fermiology and phonon dispersions. A thorough investigation of magnetism including the computation of inter-site magnetic exchanges, *q*-dependence of the interacting as well as non-interacting response functions and electron-phonon coupling matrix evince a pathway to the unresolved experimental questions like the occurrence of giant anomalous Hall effect, magnetic frustration and its inter-dependence with superconductivity, charge-order and multiple Q-nesting. In the next step, with *ab-initio* calculated inter-site exchanges as a function of the nearest neighbor distances, the magnetocrystalline anisotropy and the site projected magnetic moments, a full-fledged atomistic spin-dynamical calculation sheds light on their dynamical magnetic properties. The calculations reveal that on top of the ferromagnetic arrangement of the moments along the [001] direction, the system also hosts underlying complex landscape of spin-textures containing commensurate and incommensurate spin-spirals. The presence of such magnetic chirality along with significant DM-interactions among their non-collinear spin moments have the potential to provide a possible explanation for the experimentally observed inherent C_6 rotational and time-reversal breaking.

Pressure induced evolution of Fermi surface and de Haas-van Alphen effect in CsV_3Sb_5

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In recent years, the mathematical concept of topology has witnessed a growing recognition in describing the band structures of topological electronic materials. The quantum phenomena they exhibits (eg. flatband, nontrivial band topology, topological superconductivity, charge density wave (CDW), etc. [1-2]) are expected to hold potential for technological applications. Recently, a new prototype of kagome metals AV_3Sb_5 (A = Cs, K, Rb) are becoming center of attraction to explore intriguing interplay between CDW, superconductivity and nontrivial band topology under pressure [3,4]. In this talk, I will introduce our recent work on kagome metal CsV_3Sb_5 which is derived from a two-dimensional (2D) kagome lattice (see Fig. 1a). To understand the underlying mechanism we study the Fermi surface (FS) topology for which de Haas-van Alphen (dHvA) oscillation provides a clear picture. By varying pressure upto 45 GPa, FS as well as dHvA frequencies varies significantly. The observed fluctuations in dHvA frequency suggest the astonishing evolution of FS indicating major effect on the extremal orbit. At ambient pressure, we found three frequencies below 1000 T from the electron pocket (α) at the M point (see Fig. 1b). The contribution of electron pocket (β) has been observed at 2 GPa (Fig. 1c) with frequency 68.15 T. This suggests the suppression of CDW at 2 GPa. At around 15 GPa, electron pocket α and the extremal orbit at Γ vanishes with emergence of new orbit from the hole pocket, confirming a Lifshitz transition. Noticeably, at 45 GPa the electron pocket at high symmetry point A vanishes (not shown).

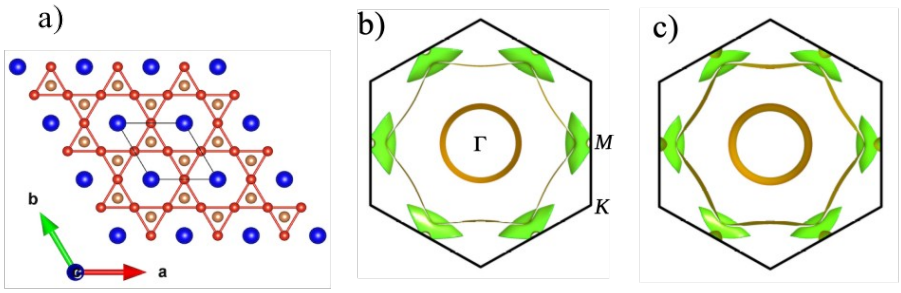

Figure 1. (a) Top view of kagome lattice of CsV_3Sb_5; 2D view of FS at (b) 0 GPa, and (c) 2 GPa.

This work was supported by a grant from UNESCO-TWAS and the Swedish International Development Cooperation Agency (SIDA).

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Asymmetric Interlayer Chalcogen Pairing Induced Type-2 Band Alignment and Energy Bandgap Reduction in Two-Dimensional Bilayer Janus SnSSe

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The inherent structural symmetry breaking in artificial two-dimensional (2D) Janus SnSSe monolayers containing two different chalcogen atoms has demonstrated unique influences on the thermoelectric [1-2], electronic [3], and optoelectronic [3-4] properties. However, to date, no systematic investigation has been attempted on any few-layer Janus SnSSe, which can potentially manifest out-of-plane asymmetry within the layers as well as between the layers [5]. Consequently, in this work, for the first time, the electronic properties of the 2D bilayer (2L) Janus SnSSe have been investigated for three distinct interlayer stacking configurations, namely S-S, Se-Se, and S-Se, based on interlayer chalcogen pairing. The key findings reveal that, unlike S-S and Se-Se, the asymmetric chalcogen pairing of S-Se in 2L-SnSSe results in asymmetric valence electron cloud overlap between S ($3s^2$ $3p^4$) and Se ($3d^{10}$ $4s^2$ $4p^4$). This further led to notable interlayer electron transfer from the top to bottom SnSSe layer, responsible for a built-in electric field development in the out-of-plane direction from the top to bottom SnSSe layer. Consequently, the relatively larger electrostatic potential at the top layer brings its conduction band minima (CBM) closer to the Fermi level, and simultaneously valence band minima (VBM) of the bottom layer shifts closer to the Fermi level. This leads to a unique type-2 band alignment between the top and bottom layer of the homogenous bilayer of SnSSe, and a notable energy bandgap reduction (~17% - 21%) in S-Se interlayer stacking configurations compared to S-S and Se-Se interlayer stacking configurations. In essence, the results suggest immense promise for interlayer stacking engineering in 2L-SnSSe for electronic/optoelectronic applications.

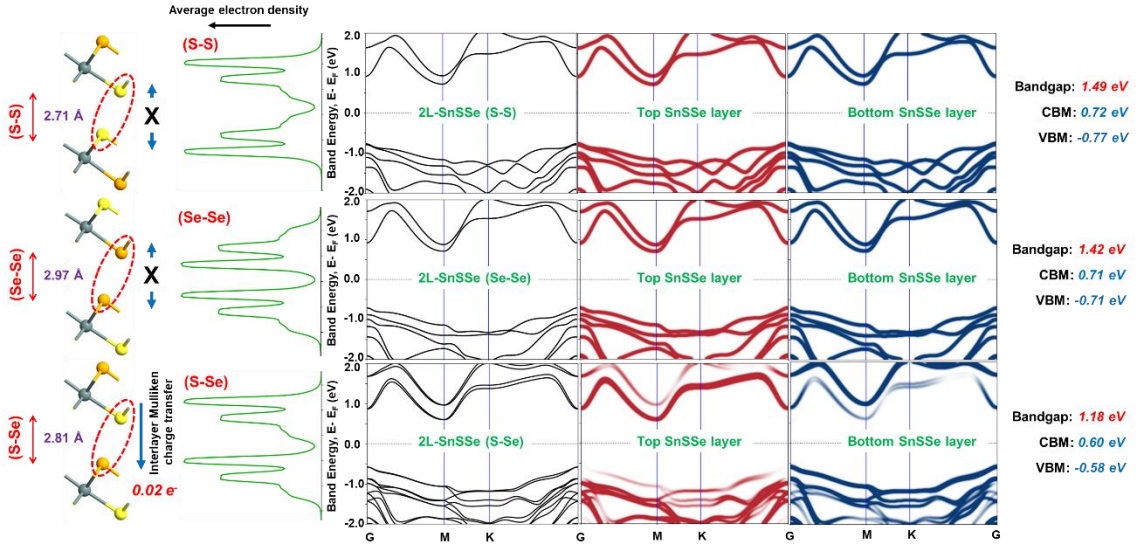

Figure 1. Plots of unit-cell schematics, average electron density, energy band structure, and layer pr ojections on energy band for 2L-SnSSe in S-S, Se-Se, and S-Se interlayer stacking configurations.

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Excitons and Exciton-Phonon Coupling in Organic-2D material Heterostructures

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Organic-2D material heterostructures are of fundamental interest because of their potential applications in photovoltaic and flexible device applications. In this work, we elucidate the nature of excitons in a prototypical organic-2D material system: phthalocyanines (ZnPc and NiPc) on a transition metal dichalcogenide monolayer, MoS2. Using first principles calculations within the GW-Bethe-Salpeter approach, we show that the excitons in these systems have a rich structure, including not only the intramolecular excitons, but also intermolecular excitons mediated by substrate interactions, and long-lived charge transfer excitons. The latter are predicted to be viable candidates for Bose-Einstein condensation at ~50-100 K [1]. We further show that the intramolecular exciton couples to the C-N-C backbone stretching phonon mode of the molecule, leading to strong resonant Raman effects, especially for NiPc on MoS2. Interestingly, many-body interactions including electron self-energy effects and electron-hole interactions in the exciton contribute significantly to the enhanced resonant Raman intensities for NiPc on MoS2. Our results are compared with time-resolved pump-probe experiments for ZnPc on MoS2 [2], and Raman intensity measurements for NiPc and ZnPc on MoS2 [3].

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3D Twistronic Photogalvanic Effect - A New Paradigm of Light-Matter Interaction in a Twisted Coordinate Frame

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We will start by discussing nonlocal photogalvanic spectroscopies where the photon momentum of engineered optical beams can be utilized to probe quantum materials (e.g., Weyl semimetals, excitonic insulators and supertwisted spirals of 2D materials) uncovering new aspects of light-matter interactions. Specifically, we will discuss the nonlinear optical Hall effect in self-assembled supertwisted multilayered WS_2 system formed by a screw-dislocation-driven mechanism. The optical Hall current direction changed with the structural handedness of the supertwisted system, along with an unusual photon-momentum dependence of the nonlinear optical response in the moire potential was observed. The observation of the nonlinear optical Hall current direction dependent on structural helicity is significant because the valley Hall associated response in 2D hexagonal lattice materials is understood to originate from the underlying Berry curvature that carries an opposite sign for the two valleys. The dependence of the optical Hall response on structural helicity is surprising, which motivated our new theoretical formalism of the anomalous transport in the multilayered supertwisted systems based on the quantum geometric formulation. Furthermore, signatures of thickness-dependent exciton-polaritons and the associated strong photon momentum-lattice interaction dependent photocurrent response were measured, which suggest a fundamentally altered light-matter interaction in 3D moire systems. Our response function theory can explain the origin of the photon momentum dependent nonlinear response, revealing new observables of the system going beyond Berry curvature and other conventional band geometrical quantities. Our study seamlessly connects 2D and 3D twistronics and provides a bridge connecting the electrons and photons by overcoming their significant length scale differences in conventional systems. These measurements also demonstrate the versatility of 3D moire systems for exploring new aspects of light–matter interaction phenomena in condensed matter systems, which are important in realizing extreme large optical nonlinearities for a variety of quantum and classical photonic applications.

Spin-orbit coupling enhanced valley ordering and orbital magnetism in twisted bilayer graphene

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Twisted bilayers of graphene (tBLG) offer a new experimental platform where interlayer Coulomb interactions play a dominant role. The formation of extremely flat bands at certain 'magic' angles, where the Coulomb energy exceeds the bandwidth, has led to the observation of correlated insulating states, superconductivity and other exotic states such as Chern insulators, orbital ferromagnets, and nematic phases. The dielectric environment of tBLG can play an important role in controlling electronic correlations within the flat bands. In this talk, I will discuss magneto-transport measurements in tBLG coupled to a layer of tungsten diselenide (WSe_2). Below half-filling, we report anomalous Hall effect with a giant coercive field, accompanied by a series of Lifshitz transitions that are highly tunable with carrier density and magnetic field. We infer that the observed valley ordering is favored by a Stoner-like instability, aided by van Hove singularities in the malleable tBLG bands. Overall, our results suggest that transition metal dichalcogenide-dielectrics can be a promising pathway to further understand and explore the nature of correlated phases in moire systems.

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Using Graphene and 2D Topological Insulators as a Global Standard for Quantum Electrical Units

Albert F. Rigosi[1*], Ngoc Thanh Mai Tran[1,2], Jason M. Underwood[1], Alireza R. Panna[1], Shamith U. Payagala[1], Randolph E. Elmquist[1], Dean G. Jarrett[1], and David B. Newell[1]

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Since 2017, epitaxial graphene has been the base material for the US national standard for electrical resistance. Due to a relaxed magnetic field and temperature requirement, these graphene-based devices enabled more user-friendly access to the quantum Hall effect and could more easily be deployed into US and global industries compared to GaAs-based devices [1]. A future avenue of research within electrical metrology is to remove the need for strong magnetic fields, as is currently the case for devices exhibiting the quantum Hall effect. New materials, like magnetically doped topological insulators, offer access to the quantum anomalous Hall effect, which in its ideal form, could become a future resistance standard needing only a small permanent magnet to activate a quantized resistance value [2]. Furthermore, these devices could operate at zero-field for measurements, making the dissemination of the ohm more economical and portable. Here we present results on precision measurements of the quantized plateau of both graphene and Cr-Doped $(Bi_xSb_{1-x})_2Te_3$. Ultimately, these devices could be combined in a single system with Josephson voltage standards to obtain an alternative quantum current standard.

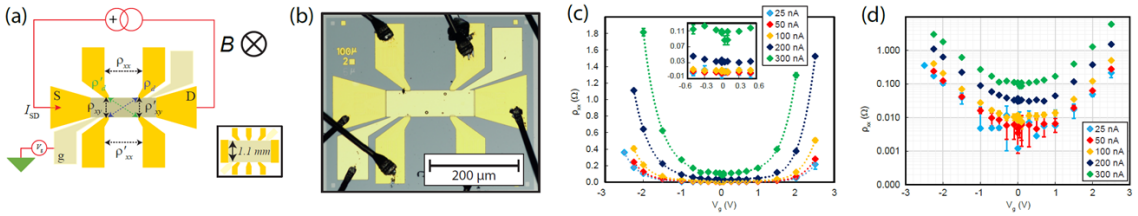

Figure 1. Fabrication of a topological insulator-based device and characterization of the longitudinal resistance.

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Detection of nontrivial topology driven by charge density wave in a layered semi-Dirac metal

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The presence of electron correlations in a system with topological order can lead to exotic ground states. Considering single crystals of $LaAgSb_2$ which has a square net crystal structure, one finds multiple charge density wave transitions (CDW) as the temperature is lowered. We find large planar Hall (PHE) signals in the CDW phase, which are still finite in the high temperature phase though they change sign. Optimising the structure within first-principles calculations, one finds an unusual chiral metallic phase. This is because as the temperature is lowered, the electrons on the Ag atoms get more localized, leading to stronger repulsions between electrons associated with atoms on different layers. This leads to successive layers sliding with respect to each other, thereby stabilising a chiral structure in which inversion symmetry is also broken. The large Berry curvature associated with the low temperature structure explains the low temperature PHE[1]. At high temperature the PHE arises from the changes induced in the tilted Dirac cone in a magnetic field[2]. Our work represents a route towards detecting and understanding the mechanism in a correlation driven topological transition through electron transport measurements, complemented by ab-initio electronic structure calculations.

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WEDNESDAY, 22 November, 2023		
Session 7A, GBR, Session Chair: Akshay Naik		
7A-1	09:00-09:30	**[Keynote] Hyeonsik Cheong** Optical Spectroscopy of Twisted Transition Metal Dichalcogenide Heterostructures
7A-2	09:30-10:00	**[Invited] Akshay Singh** Creating and measuring useful defects in 2D semiconductors
7A-3	10:00-10:15	**[Contributed] Atikur Rahman** Effect of Dielectric Environment on the Optoelectronic Properties of Mixed-Dimensional van der Waals Heterostructures
7A-4	10:15-10:30	**[Contributed] Mayank Chhaperwal** >10 MHz emission rate from monolayer-based single photon emitter array
Session 7B, Lalit 1-2, Session Chair: Alexey Berdyugin		
7B-1	09:00-09:30	**[Invited] Denis Bandurin** Teratronics in the flatland: recent advances and novel applications
7B-2	09:30-10:00	**[Invited] Mayank Shrivastava** Two-Dimensional Materials: Technological Challenges Ahead
7B-3	10:00-10:15	**[Contributed] Krishna Prasad Maity** Opto-electronic neuromorphic devices based on van der Waals ferroelectric heterostructures
7B-4	10:15-10:30	**[Contributed] Chithra H. Sharma** Addressing the mini-bands in MoS2 moiré superlattices
Session 7C, Lalit 3-4, Session Chair: Bharti Singh		
7C-1	09:00-09:30	**[Invited] Adarsh K. V.** Photoexcitation on low dimensional semiconductors and bulk single crystals: A playground for optical properties
7C-2	09:30-10:00	**[Invited] Andrea Capasso** Optimized production techniques for 2D crystal-based technology
7C-3	10:00-10:15	**[Contributed] Ramesh Rajarapu** Phase selective Synthetic 3R phase sword like MoS2
7C-4	10:15-10:30	**[Contributed] Manasi Mandal** Precise Fermi-level engineering in a topological Weyl semimetal via fast ion implantation
COFFEE BREAK, 10:30-11:00		
Session 8A, GBR, Session Chair: Priya Mahadevan		

8A-1	11:00-11:30	**[Keynote] Stephan Roche** Topological Spin Transport in Quantum Materials and Entanglement
8A-2	11:30-12:00	**[Invited] Mei Yin Chou** Origin of Magic Angles in Twisted Bilayer Graphene: The Magic Ring
8A-3	12:00-12:30	**[Invited] Abir De Sarkar** DFT perspectives on valleytronics and flexible piezo-spintronics in selected functional 2D materials
Session 8B, Lalit 1-2, Session Chair: Tanuja Mohanty		
8B-1	11:00-11:30	**[Invited] Anjana Devi** New Chemical Vapor Deposition Approaches to 2D Materials
8B-2	11:30-12:00	**[Invited] Jae-Hyun Lee** Layer-engineered atomic spalling of vdW crystals
8B-3	12:00-12:15	**[Contributed] Manvi Verma** Optical and structural characterization of epitaxially grown monolayer MoS2 on miscut c-Al2O3
8B-4	12:15-12:30	**[Contributed] Daya S. Dhungana** Two Dimensional Silicene-Stanene Heterostructure
Session 8C, Lalit 3-4, Session Chair: Sajal Dhara		
8C-1	11:00-11:30	**[Invited] Aveek Bid** Tuning topological bands in graphene
8C-2	11:30-12:00	**[Invited] Alexey Berdyugin** Giant magnetoresistance of Dirac plasma in high-mobility graphene
8C-3	12:00-12:15	**[Contributed] Nitin Kumar** Kondo Resonance in Magnetic Fe Atoms Self-Assembled on Monolayer Stanene
8C-4	12:15-12:30	**[Contributed] Aniket Majumdar** Observation of Klein-Schwinger effect in ultra-high mobility graphene
LUNCH BREAK: 12:30-14:00		
Session 9A, GBR, Session Chair: Atikur Rahman		
9A-1	14:00-14:30	**[Invited] Ageeth Bol** Advanced atomic layer deposition cycle schemes for large-area synthesis of 2D transition metal dichalcogenides
9A-2	14:30-15:00	**[Invited] M. M. Shaijumon** Engineered 2-D Heterostructures for Electrocatalysis
9A-3	15:00-15:15	**[Contributed] Vijaykumar Murugan** Bandgap engineering of monolayer Mo1-xWxS2 ternary alloys grown by gas-phase CVD

9A-4	15:15-15:30	**[Contributed] H S S Ramakrishna Matte** Solution Processing of Low-dimensional Materials and Applications
Session 9B, Lalit 1-2, Focus session on Diversity in STEM and Academia, Session Chair: Shobhana Narasimhan		
9B-1	14:00-14:45	**Interactive workshop on Diversity**
9B-2	14:45-15:30	**Panel Discussion: Madhav Prasad Ghimire** (Tribhuvan University, Nepal)**, Arvind Narrain** (National Law School of India University)**, Ranjini Bandyopadhyay** (Raman Research Institute)
Session 9C, Lalit 3-4, Session Chair: Denis Bandurin		
9C-1	14:00-14:30	**[Invited] Michael Rohlfing** Intra- and inter-layer excitons of two-dimensional semiconductors on substrates and in magnetic fields
9C-2	14:30-15:00	**[Invited] Kausik Majumdar** Van der Waals heterojunctions for quantum device applications
9C-3	15:00-15:15	**[Contributed] V.S. Volkov** Giant optical anisotropy in van der Waals materials
9C-4	15:15-15:30	**[Contributed] Nitesh Singh** Stable and deterministic source of single photons in layered hexagonal boron nitride at room temperature
COFFEE BREAK, 15:30-16:00		
Industry focus session, GBR, Session chair: Rajendra Singh		
I-1	16:00-16:25	**[Invited] Deshdeep Sahadev**, Quazar Technologies Pvt. Ltd. High-end cost-effective indigenous instruments for two dimensional materials
I-2	16:25-16:50	**[Invited] Syam Parayil Venugopalan**, ASML 2D materials at the edge of device scaling engines
I-3	16:50-18:00	**Panel Discussion: Suraj Rengarajan** (Applied Materials)**, N. Sainathan** (Tata Steel)**, Rajeev Gautam** (Horiba)**, Mangesh Kulkarni** (Oxford Instruments)**, Partha Parthasarathy** (Micron Technology)

Optical Spectroscopy of Twisted Transition Metal Dichalcogenide Heterostructures

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Heterostructures of two-dimensional materials have been extensively studied as the alignment of the bands in the constituent materials allow for manipulation of optoelectronic and transport properties. The band offset between the bands is usually the most important parameter in determining the physical properties of these structures. However, as evidenced in the so-called 'magic-angle graphene' [1], the twist angle between the crystallographic directions of the two layers is an important parameter that affect the physical properties. As the twist angle between two layers of a given set of materials is varied, the phonon spectrum as well as the electronic band structure and optoelectronic properties change systematically. Furthermore, at very small twist angles, atomic-scale lattice reconstruction [2] is observed and should be accounted for in describing the physical properties of heterostructures. Recently, we found that moiré superlattices made from single layers of MoS_2 and WSe_2 with a fairly large lattice mismatch (~4.5%) exhibit a pair of torsional distortions with opposite chirality irrespective of the twist angle [3]. The whirlpool-shaped periodic lattice distortions introduce fuzziness in the Raman spectra and universal redshifts to the intralayer excitons for all twist angles. We show that both of these modulations become weaker as the twist angle increases but do not disappear, whereas they are turned off when the constituent layers are not tightly coupled. In a lattice matched (~0.24%) heterostructures of $MoSe_2$ and WSe_2, a series of moiré phonons are observed, and the low-frequency Raman spectra show a rich array of interlayer shear and breathing modes that evolve with the twist angle [4]. Furthermore, the interlayer excitons that appear strong in the twisted heterostructures with the twist angles near 0° or 60° have different energies and photoluminescence excitation spectra for the two cases, which results from different electronic structures and carrier relaxation dynamics. These results demonstrate that the details of the lattice interactions as well as the twist angle should be considered in designing heterostructure-based devices.

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[4] S. Y. Lim, *et al*., ACS Nano (2023) https://doi.org/10.1021/acsnano.3c03883.

Creating and measuring useful defects in 2D semiconductors

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Defects in two-dimensional transition metal dichalcogenides (2D-TMDs) are promising for photonics, single photon emission and quantum information. Using a combination of Raman and photoluminescence (PL) spectroscopy, we study defect formation in mechanically exfoliated monolayer MoS_2 at ultra-low accelerating voltages (3-5 kV). We correlate spectra changes to interplay of defect creation and doping effects due to electron beam [1]. We then use a novel electron irradiation technique to create low density defects, relevant for single photon emission.

We also created a series of MoS_2 monolayer samples, differently synthesized (mechanically exfoliated, oxygen-assisted chemical vapour deposition (CVD)), and with hBN encapsulation (or hBN covered). Using low-temperature PL characterization, we uncover distinct defect signatures and correlate to nature and density of defects [2]. This comprehensive understanding of defects in MoS_2 will lead to the creation of useful and high-quality isolated defects.

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Effect of Dielectric Environment on the Optoelectronic Properties of Mixed-Dimensional van der Waals Heterostructures

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Two-dimensional (2D) materials and their heterostructures have demonstrated significant potential in various modern electronic and optoelectronic devices. However, their optoelectronic properties are strongly influenced by the defects present in these materials. Additionally, the reduced dielectric screening in the out-of-plane direction makes 2D materials highly sensitive to the surrounding dielectric environment, providing a unique platform with highly tunable optoelectronic properties. The defects in the 2D materials and at the substrates are strongly influenced by the surrounding dielectric environment. Therefore, gaining an in-depth understanding of the role of defects and the dielectric environment is crucial for designing high-performance optoelectronic devices. We have developed a simple method for fabricating large-area monolayer devices using MoS_2. Due to the 2D nature of MoS_2, the Coulomb screening is less effective, and the electronic and optoelectronic properties of these heterostructures strongly depend on the local environment. To create mixed-dimensional van der Waals heterostructures, we combined an n-type MoS_2 monolayer with a p-type bulk silicon. This 2D-3D system exhibits interesting photoresponse properties. We observed that the photoresponse strongly relies on the surrounding dielectric environment, and by adjusting the dielectric constant, one can significantly enhance the photoresponse by several orders of magnitude. In our discussion, we will explore how various characterization methods such as low-frequency noise, dielectric analysis, and transient photoresponse can be employed to comprehend the impact of defects and the dielectric environment on the charge transport properties of such systems.

References

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>10 MHz emission rate from monolayer-based single photon emitter array

Mayank Chhaperwal[1], Kenji Watanabe[2], Takashi Taniguchi[3] and Kausik Majumdar[1*]

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Defect emission in monolayer WSe_2 can be tuned and enhanced with the high-strain centers induced by nanopillar arrays, which has attracted a lot of attention for deterministic Single Photon Emitters (SPEs). Unfortunately, the reported emission rate from such SPEs is significantly lower compared with competing technologies, such as III-V quantum dots. In this work, using a high-aspect-ratio nanopillar array, we demonstrate a record high emission rate (>10 MHz) while maintaining single photon purity [$g^{(2)}(0) \sim 0.196$], making 2D material-based SPEs a viable option for quantum technologies.

We achieve the same by using negative photoresist as the material to create nanopillars with a high aspect ratio (> 1.5) on a gold-coated substrate (Fig. 1a). The resist being relatively soft and having a smooth surface makes the transfer of WSe_2 monolayer on the tall pillars possible with minimal damage to the flake. The strong exciton funneling in the structure increases the emission, achieving >10 MHz collected count rate (Fig. 1b). To the best of our knowledge, this is the highest in this category, twice as much as the previous highest reported rate[1]. In addition, the gold-coated substrate helps to quench the emission away from the pillar due to non-radiative exciton transfer to the gold film, allowing us to collect the emission only from the pillar region. This helps in maintaining the SPE purity even at higher emission rates. We measured a $g^{(2)}(0)$ value of 0.196 at a count rate as high as 1 MHz (Fig. 1c).

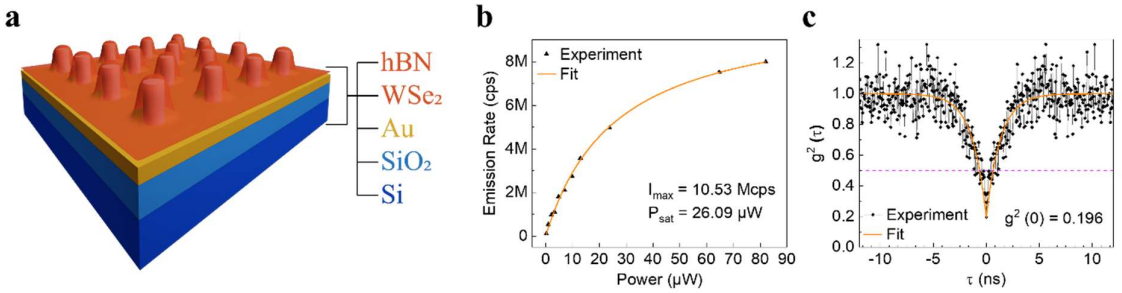

Figure 1. (a) Schematic of hBN capped monolayer WSe_2 on nanopillar array. **(b)** Integrated PL intensity (black triangles) at the collection lens for varying excitation power. Fit (orange trace) gives a maximum emission rate of 10.53 MHz. **(c)** Measured second-order correlation function (black symbols) for the SPE provides a $g^{(2)}(0)$ of 0.196. Data is fitted (orange line) with a typical $g^{(2)}(\tau)$ vs. τ curve for a 2-level system.

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Teratronics in the flatland: recent advances and novel applications

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Since the first isolation of graphene, devices based on novel low-dimensional materials (LDM) and their heterostructures have become a gold mine for exploring new fundamental phenomena. Reduced dimensionality, peculiar band structures, quantum geometry, and strong quasiparticle interactions in a unique way determine the response of LDM to external fields thereby offering a powerful setting by which to probe novel radiation-matter interaction effects and prototype future optoelectronic technology.

In the first part of my talk, we will discuss light-matter interaction effects arising in LDM due to the excitation of plasmons. I will present our recent results on the quasi-relativistic Fizeau drag effect [1]. Predicted by Fresnel in the XIX century and demonstrated by Fizeau, dragging of light by the flow of water was among the cornerstones of Einstein's special relativity. Our experiments on graphene materialized the electronic version of this fundamental effect in which the flow of electrons on par with the moving medium was found to alter the surface plasmon polaritons (SPP) dispersion (Fig. 1). The importance of the observed plasmonic Fizeau drag is that it enables breaking of time-reversal symmetry and reciprocity at infrared frequencies without resorting to magnetic fields or chiral optical pumping.

Next, we will discuss peculiar effects arising in graphene terahertz plasmonics when it is subjected to a perpendicular magnetic field. I will show that graphene supports the propagation of slow Bernstein collective modes whose diverging density of plasmonic states results in strong magnetoabsorption at THz frequencies [2]. We will also discuss prospects of using devices made of LDM for sensitive THz detection [3-5].

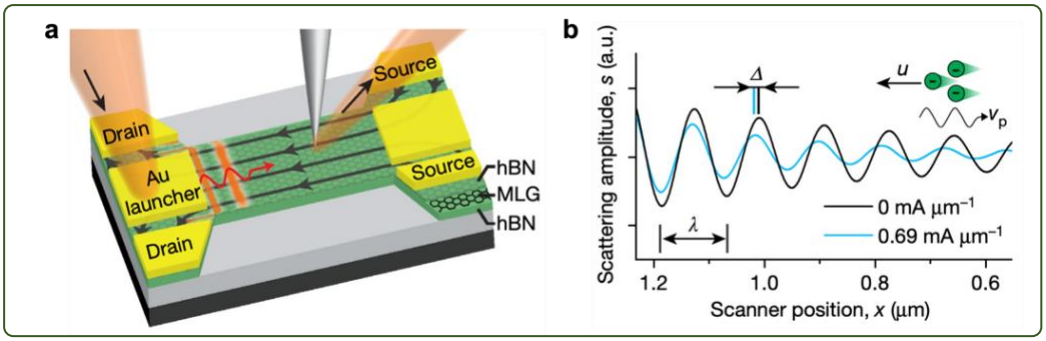

Fig. 1. Fizeau drag in graphene plasmonics. a, Schematic of a graphene device with a constricted channel. Under the illumination of an infrared laser, the gold launcher excites propagating SPPs, which were visualized by near-field tip-based imaging techniques. Black streamlines represent carrier drift directions. **b,** SPP line profiles without d.c. current (black) and with J_{dc} = 0.69 mA μm^{-1} (blue), illustrating a reduction of the SPP wavelength. Taken from [1].

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Title: Two-Dimensional Materials: Technological Challenges Ahead

Abstract: This talk will attempt to present the technological and fundamental challenges in pushing 2D technology to the market, where the world stands today, and what gaps are required to be filled. Talking about the gaps, I will particularly touch base on the Metal (3D) to graphene/TMD (2D) contact engineering challenges, which has been considered as one of the most fundamental challenges towards harnessing the full potential of 2-dimensional materials. And, how the fundamental understanding of the contact's quantum chemistry resulted in unique ways to engineer it, resulting in record transistor performance. Besides, I will talk about some of the fundamental process or process-driven reliability challenges that can unintentionally perturb the 2D channel's electrical, optical, and mechanical properties. In the end, I will talk about some of the reliability gaps, which are urgently required to be addressed, and the fundamental understanding we have developed so far.

Biography: Prof. Mayank Shrivastava is a faculty member at the Indian Institute of Science, Bangalore, and co-founder of AGNIT Semiconductors Pvt. Ltd. He is also instrumental in setting up a $60M worth of GaN prototyping Fab and leading a national effort on 2D material's technology hub. He received his Ph.D. degree from the Indian Institute of Technology Bombay (2010). For his Ph.D. work, he received the Excellence in Research award and the Industrial Impact award from IIT Bombay in 2010. He is among the first recipients of the Indian section of the American TR35 award (2010) and the first Indian to receive the IEEE EDS Early Career Award (2015). He is also an Editor of IEEE Transactions on Electron Devices. Besides, he is an IEEE Electron Device's Society (EDS) Distinguished Lecturer and an elected member of the IEEE EDS Board of Governors. He is the recipient of the prestigious DST Swarnjayanti Fellowship (2021), Abdul Kalam Technology Innovation National Fellowship from INAE-SERB (2021), and the VASVIK award (2021). He has received several other national awards and honors of high repute, like the National Academy of Sciences, India, (NASI) Young Scientist Platinum Jubilee Award – 2018; Indian National Academy of Science (INSA) Young Scientist Award - 2018; Indian National Academy of Engineering (INAE) Innovator Entrepreneur Award 2018 (Special commendation); Indian National Academy of Engineering (INAE) Young Engineer Award - 2017; INAE Young Associate (since 2017); Indian Academy of Sciences (IASc), Young Associate, 2018 – 2023; Ministry of Electronics & Information Technology (MeitY), Young Faculty Fellowship. Besides, he received best paper awards from several international conferences like the Intel Corporation Asia academic forum, VLSI design Conference, and EOSESD Symposium. Prof Shrivastava broadly works on applications of emerging materials like Gallium Nitride (GaN), atomically thin two-dimensional materials like Graphene and TMDCs, in electronic and electro-optic devices working closer to its fundamental limits (like the ability to handle extreme powers, ability to work at THz like ultra-high frequencies, or ability to compute information in unconventional ways). Currently, his group is developing few-atom thick devices & and circuits, GaN-based ultra-high-power devices with high reliability, and devices/circuits for operation at THz frequencies. Besides, his group also works on developing novel ESD and high-voltage device concepts in advanced CMOS and BiCMOS nodes, automotive, and silicon discrete technologies. He held visiting positions in Infineon Technologies, Munich, Germany, from April 2008 to October 2008 and again from May 2010 to July 2010. He worked for Infineon Technologies, East Fishkill, NY, USA; IBM Microelectronics, Burlington, VT, USA; Intel Mobile Communications, Hopewell Junction, NY, USA; Intel Corp, Mobile and Communications Group, Munich, Germany between 2010 and 2013. He joined the Indian Institute of Science as a faculty member in the year 2013. Prof Shrivastava's work has resulted in over 230 peer-reviewed publications (around 50 of these papers are in IRPS and IEDM, the two most prestigious conferences of IEEE EDS, and around 100 are in journals such as IEEE T-ED) and 55 patents. Most of these patents are either licensed by semiconductor companies or are in use in their products. More details are available at https://faculty.dese.iisc.ac.in/mayank/

Opto-electronic neuromorphic devices based on van der Waals ferroelectric heterostructures

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In the last few decades, due to the rapid development of information technology, traditional von Neumann's structure-based computing is facing the great challenges of information processing speed and high energy consumption. The human brain-inspired neuromorphic computing, where the neurons and synapses operate simultaneously by processing spikes time, shape, and magnitude, performs parallel computing and data processing, is a promising for next generation computing. Synapse is considered as the building block to mimic the human brain's analog logic, memory, and learning. Electrical control field effect transistors, memristors, and tunnel junction transistors are extensively investigated to emulate the synapse.

In this talk, I will present recent achievements in our team in developing optoelectronics neuromorphic devices taking advantage of the ultimate tunability and multifunctionality of 2D materials and their heterostructures.

1. *Optical potentiation and electrical depression:* Optoelectrical control of synapse is more promising due to their high speed and low power operations. The 2D ferroelectric and semiconductor on top exhibits synaptic functionalities, which were complemented by the unique dual optical and electrical control, enabling optically stimulated and optically assisted synaptic devices. The modulation of electrical polarization by electrical and optical stimulation creates short and long lived intermediate resistive states of the semiconductors. The wavelength-dependent study reveals ferroelectric polarization modulation mechanism driven by photogenerated carriers for each material[1].

2. *Single wavelength-controlled potentiation and depression:* All-optical control of synaptic devices[2] gives neuromorphic functionality with ultra-low power operations and is considered as potential devices for artificial visual systems due to their optical sensitivity and memory characteristics. The synaptic behaviour (with long-term and short-term potentiation and depression) of optoelectronic devices based on ferroelectric and graphene-based devices is demonstrated using single wavelength optical stimulation. The optical controlled depolarization and polarization are modulated, depending on the light pulse width and power resulting in synapse simulation of many different intermediate graphene resistive states (~200 states and more)[3].

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Addressing the mini-bands in MoS_2 moiré superlattices

Chithra H. Sharma[1,2,*], Marta Prada[1], Jan-Hendrik Schmidt[1], Tobias Stauber[3], Takashi Taniguchi[4], Kenji Watanabe[4], Lars Tiemann[1], and Robert H. Blick[1, 5]

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[2]*Christian-Albrechts-Universit ̈at zu Kiel, Leibnitzstrassee 11-19, 24098 Kiel, Germany.*
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In the last decade, the evolution of van der Waals material systems has provided a multitude of options to manipulate, control, and engineer materials properties to various needs by combination, proximity, and twisting. Moiré superlattices formed as a result of lattice mismatch or twist angle modify the electronic structure to create flat bands and host exotic correlated electron phases [1]. Unlike graphene, transition metal dichalcogenides relax the stringent magic angle condition for flat band formation [2,3].

Our transport spectroscopy measurements and analysis reveal a correlation-driven phase transition and the emergence of discrete mini-bands in MoS_2 moiré superlattices that remained elusive so far. A schematic of the twisted bilayer MoS_2 (tBLM) device encapsulated in hBN is shown in Fig. 1. We resolve these mini-bands arising from quantum mechanical tunnelling through Schottky barriers between the MoS_2 and its metallic leads. Energy scales deduced from a first approach exhibit an astounding agreement with our experimental observations. The behaviour under thermal activation suggests a Lifshitz phase transition at low temperatures that is driven by a complete spin-valley symmetry breaking. These intriguing observations bring out the potential of twisted MoS_2 to explore correlated electron states and associated physics.

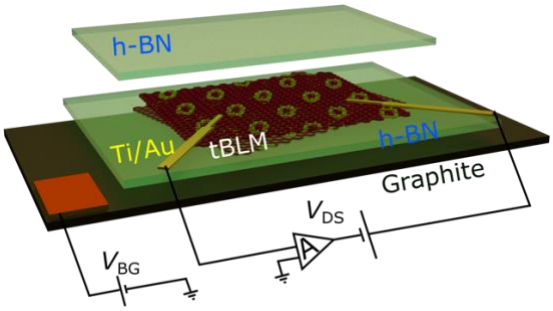

Figure 1. Schematic of the sample configuration with the MoS_2 moiré superlattices encapsulated in hBN.

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Photoexcitation on low dimensional semiconductors and bulk single crystals: A playground for optical properties

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Many-body interactions of charge carriers in quantum-confined semiconducting nanostructures are enhanced relative to their bulk counterparts and thus have opened new opportunities for manipulating and enhancing light-matter interactions. From a fundamental point of view, the enhanced Coulomb interactions due to the low dimensional confinement endow carrier-carrier interactions that are predicted to generate exotic effects such as exciton complexes, coherent optical Stark effect, Mott transitions, bandgap renormalization, and condensation of charge carriers. Here, we report the many-body interactions in the semiconducting solution processable metal halide perovskite (MHP) quantum dots (QDs) of the general formula ABX_3, the unusual coherent optical Stark effect of redshift, Autler-Townes-like splitting and blue shift as a function drive photon frequency in the framework of interacting biexciton picture, spin selective bandgap renormalization, and electron-hole liquid at room temperature. Likewise, *s*trong Coulomb interaction is one of the important keys that leads to the formation of diverse excitonic states in bulk transition metal dichalcogenide single crystals. This Coulombic interaction can be tuned by alloying their binary counterparts, which offers freedom to enhance the optical and electronic properties. However, a limited understanding of excitonic interactions and their physical origin in these alloys hinders their importance in practical applications. Here, we demonstrate diversities of excitonic features such as the high-energy A' and B' excitons in addition to the usual A and B excitons and excitonic Rydberg series in ternary $Mo_{0.5}W_{0.5}S(Se)_2$ single crystals using

temperature-dependent reflectance spectroscopy. Our experimental and theoretical studies provide a comprehensive understanding of the unresolved discrepancies in the various excitonic interactions and suggest that alloy single crystals are better materials for a wide range of optoelectronic applications.

Optimized production techniques for 2D crystal-based technology

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2D crystals (2DC) are used in a variety of applications, including energy harvesting and storage, water purification, and sensing. Sustainable and scalable production techniques are actively researched to bring 2DCs from the lab to the market. In principle, liquid phase exfoliation (LPE) methods allow for the production of 2DCs on a large scale at a reasonable cost, but in practice most of these methods are not directly upscalable and often require dangerous and toxic solvents (e.g., NMP, DMF, and DMSO).[1,2] Here, we show how to efficiently exfoliate graphite into few-layer graphene flakes by high-shear mixing in dihydrolevoglucosenone (Cyrene), an ecologically safe solvent.[2,3] Stable dispersions with 1 mg/mL concentration were used to fabricate nanofiltration membranes on PVDF supports by vacuum filtration. Transport studies with KCl, $CaCl_2$, and $AlCl_3$ ions demonstrated that the membranes operate via charge- and size-selection.[4,5] In particular, the positively charged nanochannels confer anion selectivity to the membrane. Dynamic diffusion studies with the antibacterial compound tetracycline revealed rejection rates exceeding 96%. Antimicrobial tests with *S. Aureus* and *E. Coli* bacteria strands revealed no biofilm formation and a decrease in bacterial adhesion with respect to commercial reverse osmosis membranes. Similar LPE methods can be optimized to produced stable dispersions of other 2DCs (*i.e.*, hBN and $Ti_3C_2T_x$ MXene) in Cyrene at high concentrations (up to 2 mg/mL), to target a wide range of applications. To increase the production yield of graphene from LPE, we implemented a complementary high-pressure airless spray process, reaching a lab-scale production of 1 L/h (at a typical concentration of 1.5 mg/mL). We used the graphene flakes in powder form, we produced in large amount to make a universal, eco-friendly paste with high electrical conductivity. The paste was deposited by blade coating to make coatings on various substrates, and it showed a strong adhesion and low sheet resistance (down to 7 Ω/□ for a 50-µm coating). We fabricated electrodes for interdigitated micro-supercapacitors (mSCs) on flexible PET.[6] The mSCs showed areal and volumetric capacitances of 6.16 mF cm^{-2} and 2.46 F cm^{-3}, and a Coulombic efficiency close to 100%. The maximum energy density exceeded 200 µWh cm^{-3} with 91.5% capacitance retention after 10000 Galvanostatic charge-discharge cycles. The mSCs maintained their performance under bending. The versatility of the graphene-based paste was further demonstrated by fabricating high-performance coatings for electromagnetic interference shielding and wearable strain sensors.

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Phase selective Synthetic 3*R*-phase sword like MoS_2

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Abstract:

The synthesis of materials with specific polymorphic phases in a chemical vapor deposition (CVD) process necessitates a meticulous balance among various thermodynamic variables.[1-3] In this study, we present a methodology to synthesize rhombohedral (3R) phase MoS_2 in well-defined sword-like geometry, exhibiting lengths of up to 120 µm, uniform widths ranging from 2-3 µm, and thicknesses of 3-7 nm by precisely controlling the dynamics of carrier gas flow from continuous mode to pulsed mode during the CVD growth process. To validate the formation of the 3R-phase material, we investigate its characteristic signatures. The resulting MoS_2 swords exhibit a high degree of circular dichroism (~58% at 100 K), accompanied by a distinctive evolution of low-frequency Raman peaks and an increasing intensity of second harmonic signals with increasing number of layers.[1] These findings conclusively establish the presence of the 3R phase in the material. Further, a field effect mobility of 40 cm^2/V-s and an I_{on}/I_{off} ratio of ~10^6 confirm the exceptional electronic quality of the 3R-phase MoS_2.[1] These findings hold significant promise for the advancement of emerging quantum electronic devices, valley-based physics and nonlinear optical phenomena in layered materials.

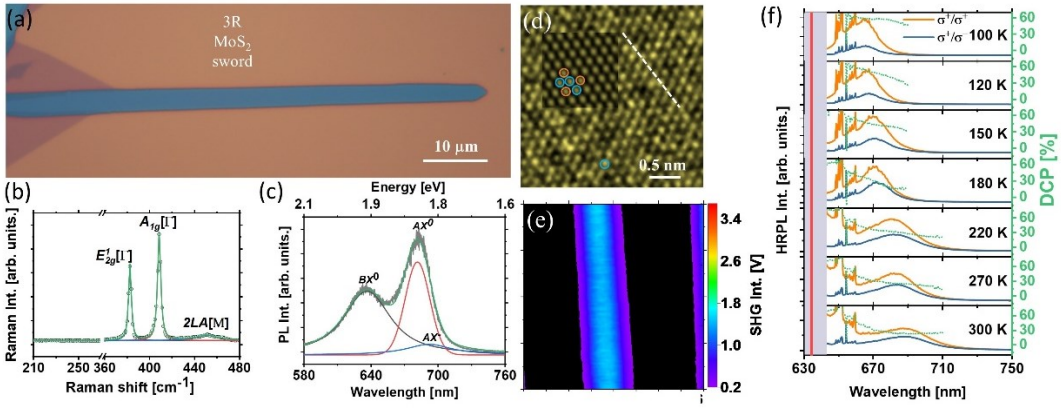

Figure 1. (a) 3R-phase of MoS_2 sword (b-c) Single point Raman and PL (d) High-resolution transmission electron microscopy (e) Second harmonic generation mapping (f) Degree of circular polarization

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Precise Fermi-level engineering in a topological Weyl semimetal via fast ion implantation

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The precise control of the Fermi level plays a crucial role in the behavior of quantum materials. While it is relatively easy to tune the Fermi level in low-dimensional materials using various techniques, the same level of control has been lacking for bulk crystals, except through chemical doping. This limitation is particularly problematic for topological Weyl semimetals, where there is a pressing need to adjust the Fermi level to match the Weyl points and unlock the divergent Berry curvature. We present a breakthrough in Fermi-level tuning for bulk Weyl semimetal TaP using high-energy hydrogen implantation facilitated by accelerators. Through this technique, we achieve ultrafine tuning of the Fermi level. Quantum oscillation measurements confirm that the Fermi level is tuned to approximately 1 meV in close proximity to the Weyl points. Our findings are further supported by density functional theoretical calculations. The significance of our approach lies in its broad applicability and high level of controllability.

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Topological Spin Transport in Quantum Materials and Entanglement

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I will present theoretical spin transport features in $MoTe_2$ and WTe_2-based materials which are particularly interesting Quantum Materials [1]. By focusing on the monolayer limit, using DFT-derived tight-binding models and using both efficient bulk and multi-terminal formalisms and techniques [2,3], I will first discuss the emergence of new forms of intrinsic spin Hall effect (SHE) that produce large and robust in-plane spin polarizations. Quantum transport calculations on realistic device geometries with disorder demonstrate large charge-to-spin interconversion efficiency with gate tunable spin Hall angle as large as $\theta_{xy}\approx 80\%$, and SHE figure of merit $\lambda_s.\theta_{xy}\sim$8-10 nm, largely superior to any known SHE material [4]. I will show our theoretical prediction of an unconventional canted quantum spin Hall phase in the monolayer T_d-WTe_2, which exhibits hitherto unknown features in other topological materials [5]. The low symmetry of the structure induces a canted spin texture in the yz plane, dictating the spin polarization of topologically protected boundary states. Additionally, the spin Hall conductivity gets quantized ($2e^2/h$) with a spin quantization axis parallel to the canting direction. We also predict the control of the canted QSHE by electric field [6]. I will finally discuss the role of entanglement between intraparticle degrees of freedom in spin transport and dynamical patterns of entanglement, as enabling novel platform for generating and manipulating quantum entanglement between internal and interparticle degrees of freedom [7].

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Origin of Magic Angles in Twisted Bilayer Graphene: The Magic Ring

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The unexpected discovery of superconductivity and strong electron correlation in twisted bilayer graphene (TBG), a system containing only *sp* electrons, is considered as one of the most intriguing developments in two-dimensional materials in recent years. The key feature is the emergent flat energy bands near the Fermi level, a favorable condition for novel many-body phases, at the so-called "magic angles". The physical origin of these interesting flat bands has been elusive to date, hindering the construction of an effective theory for the unconventional electron correlation. In this work, we have identified the importance of charge accumulation in the AA region of the moiré supercell and the most critical role of the Fermi ring in AA-stacked bilayer graphene. We show that the magic angles can be predicted by the moiré periodicity determined by the size of this Fermi ring. The resonant criterion in momentum space makes it possible to coherently combine states on the Fermi ring through scattering by the moiré potential, leading to flat bands near the Fermi level. We thus establish the physical origin of the magic angles in TBG and identify the characteristics of one-particle states associated with the flat bands for further many-body investigations.

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DFT perspectives on valleytronics and flexible piezo-spintronics in selected functional 2D materials

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Abstract

Novel properties such as piezoelectricity and valley physics arise at the nanoscale which are usually non-existent in the bulk form of the materials. HfN_2 monolayers[1] exhibit valleytronic properties complementary to that in single-layer MoS_2, while the merger of spintronic with valleytronic properties is observed in h-NbN and h-TaN monolayers[2]. Out-of-plane piezoelectricity is induced at the interfaces of 2D semiconducting planar monolayers, which show in-plane piezoelectricity individually and zero out-of-plane polarization/piezoelectricity, such as GaN and boron monophosphide (BP) monolayers. The understanding reached in GaN/BP van der Waals heterobilayers (vdWHs) has been reinforced on MoS_2/BP and MoSSe/BP vdWHs. Experimental verification of these theoretical predictions is encouraging. The origin of negative piezoelectricity at the interfaces of 2D dialkali oxide and chalcogenide monolayers has been elucidated together with the enhanced electrical conductivity arising from nearly free electron gas (NFEF) states[3]. The conflux of tunable Rashba effect and piezoelectricity observed in flexible MgTe, CdTe, and ZnTe monolayers signify its super high prospects for self-powered flexible-piezo-spintronics[4]. The nature of metal-semiconductor contacts plays a crucial role in determining device performance. Non-resistive/Ohmic contact is found to occur in graphene/MgS vdWH, rendering it ideal for charge injection[5].

Keywords: piezoelectricity; flexible piezo spintronics; valleytronics, 2D materials

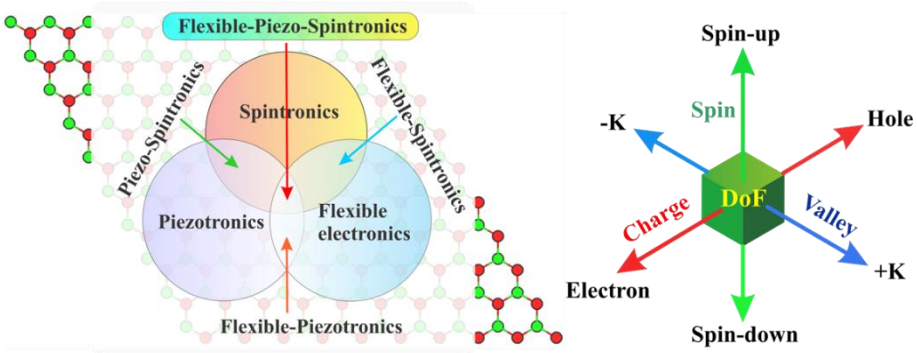

Fig. 1: Schematic representation of the abstract

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New Chemical Vapor Deposition Approaches for 2D-Materials

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Functional 2D materials have shown bright prospects in broad application fields including microelectronics, spintronics, optoelectronics, lithium batteries, hydrogen storage, gas, and biosensors etc. For future industrial innovations, from two-dimensional material (2D) on wafer size to large-scale integrated circuit fabrication is currently a big challenge. Compared to the top-down methods, the bottom-up approach of synthesizing 2D materials has a wider application scope. Chemical vapor deposition (CVD) and atomic layer deposition (ALD) routes are favorable due to their scalability, and they are industrially compatible. For 2D-TMDCs such as molybdenum (MoS_2) and tungsten disulfides (WS_2), metalorganic chemical vapor deposition (MOCVD) and ALD routes employing tailored precursors enables processing crystalline and high-quality layers at moderate temperatures unlike the classical CVD process where the sulfurization of metal oxides need high temperatures or post-deposition treatment. In this presentation, new precursor chemistry combinations are discussed that enable the direct growth of high quality, large-area crystalline and stoichiometric TMDCs, thus circumventing the post-deposition annealing process. Studies on the nucleation and growth of the layers on various substrates revealed different growth modes and nucleation density. A comprehensive analysis of the MoS_2 and WS_2 layers demonstrates the strong impact of the process parameters including the role of precursors. This enables tuning of material properties for functional applications. This presentation will give a first insight on the new avenues for the fabrication of TMDCs.

Layer-engineered atomic spalling of vdW crystals

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Abstract:

Two-dimensional materials (2DMs) have been intensively studied for almost two-decade since the isolation of graphene from bulk graphite into devices in 2004. Over the past few years, the utilization of 2DMs in various areas of industry has strongly intensified. However, even though considerable efforts have been spent on the development of various methods of the production of 2DMs, the efficient production of 2DMs of a guaranteed quality over a large scale remains a challenge. In this seminar, I am going to introduce atomic spalling of the van der Waals crystals that achieve large area 2DMs (graphene, MoS_2, $MoSe_2$, and WSe_2) with a controlled number of layers [1]. We found that being a layered crystal with a weak interlayer vdW force enables to control of the crack propagation depth at the scale corresponding to the single atomic thickness by adjusting interfacial toughness and the internal stress of the stressor film. The presented results show huge potential for the manufacture of layer-resolved high-quality vdW materials, which can be developed into practical functional electronic and photonic devices.

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Optical and structural characterization of epitaxially grown monolayer MoS_2 on miscut c-Al_2O_3

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Transition metal dichalcogenide (TMD) monolayers and heterostructures are an important class of 2D materials, particularly promising for semiconductor and opto-electronic applications[1]. Crystalline substrates such as sapphire (Al_2O_3), serve as an excellent platform for realizing large area, single crystalline growth of TMDs, guided by symmetry of the underlying lattice[2]. These substrates usually feature step edges which are dependent on the specified miscut angle and direction from the primary axis and can lead to strain in the as-grown aligned flakes. Moreover, coalescence of nearly aligned neighboring grains can lead to the formation of low angle grain boundaries (LAGBs), due to slight crystallographic misorientation[3].

We have used chemical vapor deposition (CVD) to grow single crystal monolayer MoS_2 flakes on annealed crystalline sapphire (c-Al_2O_3) by van-der-Waals epitaxy. The as-grown flakes were confirmed to be monolayer MoS_2 by optical microscopy, Raman and photoluminescence spectroscopy. Further, we have carried out polarization dependent optical measurements to characterize the strain in such samples due to the presence of underlying Al_2O_3 substrate. Polarization dependent Raman spectra of MoS_2 grown on Al_2O_3 featuring different miscuts from the primary c-axis were compared with exfoliated MoS_2. Finally, the CVD grown flakes were transferred to a TEM grid by a polymer assisted wet transfer technique. Scanning transmission electron microscopy (STEM) was performed for atomic scale characterization of the transferred flakes. STEM images directly show the lattice structure, as well as the presence of defects and grain boundaries at the site of coalescence of two neighboring grains. We have explored the significant influence of substrate symmetry and miscut angle on the nature of strain and coalescence in CVD grown monolayer MoS_2.

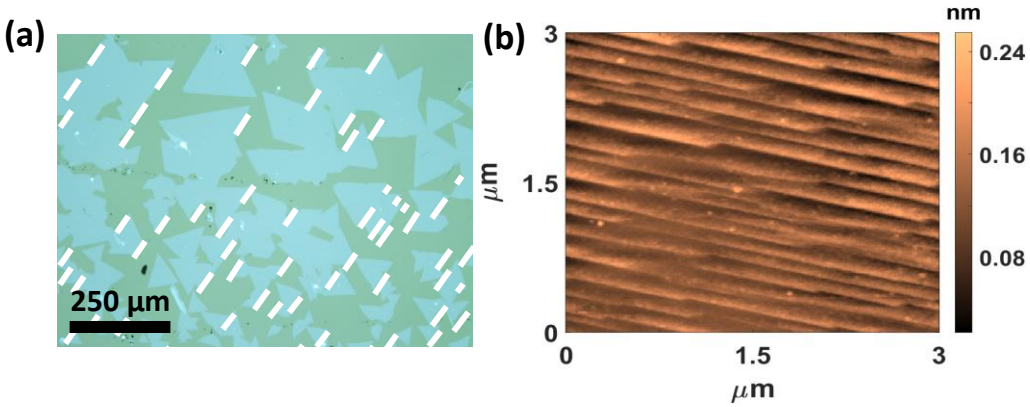

Figure 1. (a) Epitaxial growth of monolayer MoS_2 on c-Al_2O_3.The dashed lines indicate the direction parallel to step edges on annealed Al_2O_3 substrates. (b) AFM image of the same substrate showing a step and terrace morphology

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Two Dimensional Silicene-Stanene Heterostructure

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The debut of graphene-like two-dimensional (2D) silicon, i.e. Silicene, in the past decade has opened the path for a variety of potential applications in the field of like nanoelectronics, energy and nano-optics. Although the Silicene fabrication process is well established in the literature, few existing bottlenecks need to be met to preserve and transfer their peculiar properties to devices. First, the monolayer Silicene that is grown on pristine Ag(111) by Molecular Beam Epitaxy (MBE) appears as a mixture of 4×4, √13×√13 R13˚ type-I and II, and other reconstructions. Second, when multilayer Silicene is realized by piling additional atomic Silicene layers on the first monolayer, the Silicene superstructures show single √3×√3 R30˚ reconstructions but are with multiple rotational domains.[1]

An appealing way to address this concern is to engineer the Silicene growth via '2D Silicene-Stanene Heterostructure' with substrate modification that we recently showed.[2] With this concept, it is possible to use epitaxial Stanene as a buffer layer over Ag(111), where single-phase Silicene, whether mono or multilayer, can be realized.[3] Furthermore, the growth of Silicene can be modulated with epitaxial Sn coverage, where partial coverage yields single-phase 4x4 and full coverage yields √3x√3 R30˚ Silicene phases for monolayer. Thus, the issue of multiple phases coexisting was completely mitigated. All these outcomes, along with the reversed configuration, will be presented and discussed in detail with various in-situ and ex-situ characterizations and in terms of theoretical studies.

In addition, some of the recent and promising consequences of aforementioned single phase Silicene via crystal phase engineering on Sn modified Ag(111) substrate, for instance, (i) realization of bendable Silicene membranes,[4] (ii) prevention of Silicene degradation and (iii) optical and thermal responses of Silicene[5] will be presented and discussed in detail. These findings paved a way to introduce other graphene-like materials in the heterostructure configuration, our recent results of introducing 2D Bismuth (Bi) layer on similar and engineered Ag(111) substrate will also be highlighted.

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Recently, there has been a surge of interest in the topological phases of matter, both experimentally and theoretically. The interest in this field stems from the fact that these phases are robust against perturbations, with the caveat that these perturbations reserve certain symmetries. Current efforts have focused on investigating the properties of discovered topological phases and the experimental realization of theoretically predicted but undiscovered phases. A few examples of topological phases being studied are the topological insulator, topological superconductor, Quantum anomalous Hall insulator (QAHI), Quantum Spin Hall insulator, and Quantum Valley Hall phases. At the phase transition, new topological phases exist, such as Dirac or Weyl semimetal, depending on the system's symmetries. Topological phases can also be introduced by breaking the symmetries of the system with external perturbations like electric and magnetic fields. Proximity-induced effects introduced by stacking with other materials are another approach that can be used for a similar outcome.

We are interested in the ability to induce transitions (either optically or electrically) between topologically non-trivial and trivial states in graphene. This is best achieved by controlling the band structure of graphene. I will discuss two approaches we have taken in our research group to achieve this – (1) proximitizing graphene with materials possessing desirable properties[1,2] and (2) modulating the graphene lattice itself. I will provide examples of each approach and discuss the (possible) future directions this research will take

Abstract.
The most recognizable feature of graphene's electronic spectrum is its Dirac point, around which interesting phenomena tend to cluster. At low temperatures, the intrinsic behaviour in this regime is often obscured by charge inhomogeneity but thermal excitations can overcome the disorder at elevated temperatures and create an electron–hole plasma of Dirac fermions. The Dirac plasma has been found to exhibit unusual properties, including quantum-critical scattering and hydrodynamic flow. However, little is known about the plasma's behaviour in magnetic fields. Here we report magnetotransport in this quantum-critical regime. In low fields, the plasma exhibits giant parabolic magnetoresistivity reaching more than 100 per cent in a magnetic field of 0.1 tesla at room temperature. This is orders-of-magnitude higher than magnetoresistivity found in any other system at such temperatures. We show that this behaviour is unique to monolayer graphene, being underpinned by its massless spectrum and ultrahigh mobility, despite frequent (Planckian limit) scattering. With the onset of Landau quantization in a magnetic field of a few tesla, where the electron–hole plasma resides entirely on the zeroth Landau level, giant linear magnetoresistivity emerges. It is nearly independent of temperature and can be suppressed by proximity screening, indicating a many-body origin. Clear parallels with magnetotransport in strange metals and so-called quantum linear magnetoresistance predicted for Weyl metals offer an interesting opportunity to further explore relevant physics using this well defined quantum-critical two-dimensional system.

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Kondo Resonance in Magnetic Fe Atoms Self-Assembled on Monolayer Stanene

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Atomic-scale spin entity in a two-dimensional topological insulator lays the foundation to manufacture magnetic topological materials with single atomic thickness. Here, we have successfully fabricated Fe monomer, dimer and trimer on the monolayer stanene/Cu(111)[1] through a low-temperature growth and systematically investigated Kondo effect by combining scanning tunneling microscopy/spectroscopy (STM/STS) with density functional theory (DFT) and numerical renormalization group (NRG) method. Given high spatial and energy resolution, tunneling conductance (dI/dU) spectra have resolved zero-bias Kondo resonance and resultant magnetic-field-dependent Zeeman splitting, yielding an effective spin S_{eff} = 3/2 with an easy-plane magnetic anisotropy on the self-assembled Fe atomic structures. Reduced Kondo temperature along with attenuated Kondo peak amplitude from Fe monomer to trimer have been further identified as a manifestation of Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between Sn-separated Fe atoms. Such magnetic Fe atom assembly in turn constitutes important cornerstones for developing local magnetism on the single-atomic-layer stanene with nontrivial band topology.

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Refrigeration of hydrodynamic electrons below lattice temperature in ultra-high mobility graphene heterostructures

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Graphene-based 2D van der Waals (vdW) heterostructures have proven to be a promising alternative to replace silicon in nanoscale electronic devices and integrated circuits in the last decade. But miniaturization of these solid-state devices to the nanoscale regime poses significant challenges in terms of heat dissipation. Shrinking device dimensions increases the density of heat generation, leading to localized thermal hotspots that can degrade device performance, and reliability, and even cause device failure. Recent efforts in this research direction have explored cooling mechanisms for graphene hot electrons via supercollisions [1], acoustic phonon-mediated scattering [2] and hBN-mediated phonon-polaritons [3,4]. In this work [5], we demonstrate a novel refrigeration mechanism in ultraclean graphene devices (mobility > 10^5 $\mathrm{cm}^2 V^{-1} \mathrm{s}^{-1}$) that is able to cool down hot electrons to almost 30 K below the lattice temperature. Using Johnson noise thermometry [6], we measure the electronic temperature across the graphene channel under different applied current biases, and observe electronic cooling below the lattice temperature at high bias currents, despite the transfer characteristics displaying the usual temperature dependence. This refrigeration mechanism is sensitive to carrier densities very close to the Dirac point of graphene and a lattice temperature range of $60 - 120$ K. Our current theoretical understanding points towards a process dominated by hydrodynamic electron-electron interactions, leading to hot electrons tunnelling through the gold-graphene junction into the electrodes.

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Advanced atomic layer deposition cycle schemes for large-area synthesis of 2D transition metal dichalcogenides

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2D materials have been the focus of intense research in the last decade due to their unique physical properties. This presentation will highlight our recent progress on the large-area synthesis of two-dimensional transition metal chalcogenides for nanoelectronics using advanced atomic layer deposition cycle schemes. First, I will discuss how we can use advanced cycle schemes to deposit wafer-scale polycrystalline MoS2 thin films at very low temperatures down to 100 °C. We have identified the critical role of hydrogen during the plasma step in controlling the composition and properties of molybdenum sulfide films. By increasing the H2/H2S ratio or adding an extra hydrogen plasma step to our ALD process, we are able to deposit pure polycrystalline MoS2 films at temperatures as low as 100 °C. To the best of our knowledge, this represents the lowest temperature for crystalline MoS2 films prepared by any chemical gas-phase method.[1]

ALD-grown 2D films tend to exhibit a high density of out-of-plane 3D structures in addition to 2D horizontal layers. While the out-of-plane 3D structures are ideal for catalysis applications, the presence of such 3D structures can hinder charge transport, which hampers device applications. In this presentation I will show how we used mechanistic insight obtained by HRTEM to tune the shape and density of the 3D structures during plasma-enhanced ALD using advanced atomic layer deposition schemes. The obtained morphology control was further confirmed by electrical measurements.[2]

Earlier [3] we have shown that ALD is an excellent technique to make MoxW1-xS2 alloys with precise control over the alloy composition. Here, I will focus on how (plasma-enhanced) atomic layer deposition can aid in synthesizing doped 2DTMCs with precise control over the doping concentration by using elaborate ALD dosing schemes.

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Engineered 2-D Heterostructures for Electrocatalysis

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Atomically thin layered transition metal dichalcogenides (TMDs) such as MoS_2, WS_2, $MoSe_2$ and WSe_2 have been emerging as the cutting edge in materials science and engineering, due to their interesting electronic properties.[1] These materials open up new opportunities for a variety of applications, including optoelectronics, energy conversion, and catalysis. To realize their potential device applications, it is highly desirable to achieve controllable growth of these layered nanomaterials, with tunable structure and morphology. TMDs exhibit promising catalytic properties for hydrogen generation and several approaches including defect engineering have been shown to increase the active catalytic sites.[2,3] The talk will present some of our efforts on morphological and electrocatalytic studies of engineered 2D nanomaterials and their heterostructures.[4-6] For instance, our recent studies on one-step chemical vapor deposition growth of Se/WSe_2 heterostructures and strain-engineered TMDs towards efficient electrocatalytic hydrogen evolution reaction will be covered.

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Bandgap engineering of monolayer $Mo_{1-x}W_xS_2$ ternary alloys grown by gas-phase CVD

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Two-dimensional (2D) transition metal dichalcogenides (TMDs) are attractive due to their unique thickness dependent optical and electrical properties. This makes them as potential candidates for optoelectronic, electronic, spintronic and catalysis applications. The band gap of TMDs is limited in the binary MoS_2 and WS_2 platforms. Engineering the bandgap in TMDs would result a larger wavelength emission region, which is essential for optoelectronic applications. Herein, we synthesized $Mo_{1-x}W_xS_2$ ternary alloys with precise composition control by gas-phase chemical vapor deposition. The compositions was tuned for the entire range of x from 0 to 1. Moreover, we observed three different phase formation with respect to the changing of W substitution in the MoS_2 lattice utilizing photoluminescence and optical absorption spectroscopy. PL spectra reveals an overall emission energy tuning of 185 meV via lattice strain, structural defects and alloying effect[1]. A lattice tensile strain of ~0.8% was estimated when the W atom substituted in the MoS_2 lattice calculated utilizing Raman spectropy. Furthermore, the existence of point and line defects determined by the HRTEM images and line profiles shows the presence of Mo and W atoms in the $Mo_{1-x}W_xS_2$ lattice[1].

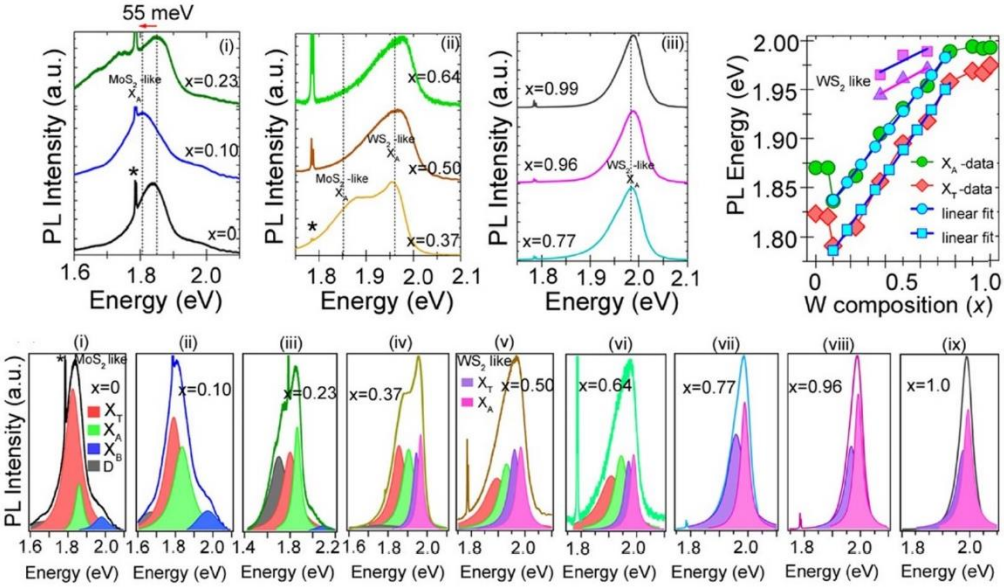

Figure 1. PL spectra of $Mo_{1-x}W_xS_2$ monolayer alloy with three different phase region and exciton and trion peak positions.

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Solution Processing of Low-dimensional Materials and Applications

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Low-dimensional Materials like graphene, transition metal dichalcogenides, h-BN, transition metal oxides and layered double hydroxides possess the potential for applications across various fields. Liquid phase exfoliation of these layered crystals enables the solution processing of dispersions of mono- and few-layers, and provides a scalable viable alternative to other physical and chemical routes. The quality of the dispersions and their applicability are dependent on the exfoliation and stabilization of the exfoliated material by the solvent, often chosen on the basis of Hansen solubility parameters (HSP). In this work, the factors at play in liquid phase exfoliation besides HSP are explored via various experimental methods, in order to further enhance the versatility of the process by providing a deeper insight. By considering molecular aspects of the solvents, highly concentrated nanosheet dispersions were obtained in a low boiling point solvent. I will also discuss about experimental determination of the HSP of layered materials. I will be concluding my talk by discussing some of our recent efforts in exfoliating non-layered materials and applications of the 2D dispersions in various fields like flexible electronics, energy storage/conversion devices and electrochemical biosensors.

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Intra- and inter-layer excitons of two-dimensional semiconductors on substrates and in magnetic fields

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Excitonic states in two-dimensional semiconductors, in particular in transition-metal dichalcogenides (TMDC), exhibit characteristic optical properties combining spin selectivity with reduced dimension. They can be described by standard many-body perturbation theory (MBPT), notably by the GW method in combination with the Bethe-Salpeter equation. Due to their low-dimensional structure, the excitons in these systems can easily be manipulated and tuned by external stimuli. Here we discuss in particular (i) energetic red-shifts of TMDC monolayer excitons due to a supporting substrate [1], (ii) the layer dependence of polarizability-related shifts at TMDC surfaces [2], and (iii) magnetic-field induced shift and splitting of intra- and inter-layer excitons [3,4,5,6].

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Van der Waals heterojunctions for quantum device applications

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Van der Waals heterojunctions allow us to manipulate electrons at the atomic scale. In this talk, I shall discuss probing discrete electron fluctuation in an electrically creat ed quantum dot using such heterojunction. I shall show the application of the same in two interesting on-chip quantum devices, namely, (a) high quality, all-electronic rando m number generator with near-ideal min-entropy, and (b) room-temperature single phot on detector @1550 nm with efficiency >20%.

Giant optical anisotropy in van der Waals materials

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Materials with high optical anisotropy are of great importance in technology and science [1]. Recently, one of the largest birefringence in the visible and near-infrared intervals up to 0.8 was reported in quasi-one-dimensional crystal $BaTiS_3$ [2]. However, anisotropic nanophotonics requires optical anisotropy of about 1.5 to fully exploit advantages of anisotropic properties [3, 4]. Inspired by this challenge, we focused on two-dimensional materials and their bulk counterpart – van der Waals (vdW) materials. Our findings showed that their fundamental difference between interlayer strong covalent bonding and interlayer weak van der Waals interaction leads to unprecedented high birefringence with values exceeding 1.5 in the infrared and 3.0 in the visible spectral intervals (for example, see optical constants of MoS_2 in Figure 1). Thus, our studies enable a new field of vdW anisotropic nanophotonics.

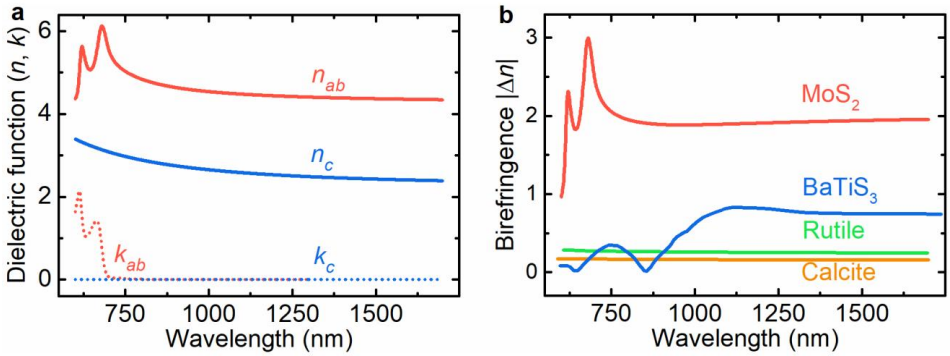

Figure 1: a. Optical constants of MoS_2. **b.** Birefringence of MoS2 in comparison with other anisot ropic materials.

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Stable and deterministic source of single photons in layered hexagonal boron nitride at room temperature

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Presence of sub-bandgap solid state point defects in high-bandgap semiconductor materials has shown significant promises in the last few decades to control the light properties even at the level of single photons. [1-3] Here, we study the quantum optical properties of a photostable, site-specific and isolated sub bandgap point defect center in layered hexagonal-boron nitride (h-BN) at room temperature. Low-energy electrons irradiation and subsequent annealing at high temperature paves the way to achieve such stable quantum emitters. Scanning confocal images confirm the presence of deterministic, isolated, bright quantum emitter with distinct zero-phonon line at 578 nm accompanied by well-separated phonon side band at 626 nm. The estimated Debye-Waller factor is more than 60% which corresponds to very low Huang-Rhys value below unity. This indicates the minimal electron-phonon interaction involved in the emission process. Moreover, the second-order intensity-intensity correlation measurement shows an anti-bunching dip of ~0.25 at τ=0, implies the definite source of single photon. Additionally, linear polarisation dependent optical properties of the quantum emitter is studied to unravel the intricate dipolar behaviour of the defect states. Therefore, our results emphasize the precise detection and control of single, isolated, and photo-stable quantum emitter using few layers of h-BN at room temperature, which might be useful for the quantum technology application

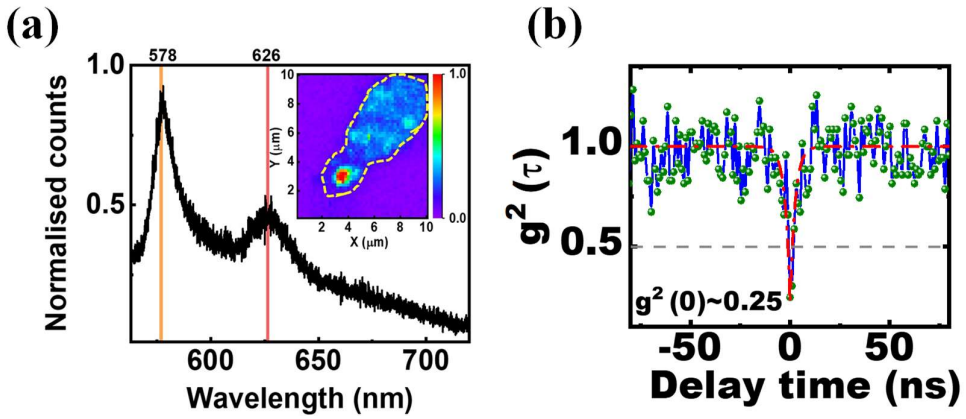

Figure 1. (a) Normalized emission spectra depicts the presence of prominent ZPL related transition (orange line) along with the broader PSB emission (red line), red shifted by ~ 165meV. The inset shows the confocal image of few layer h-BN flake (yellow dotted line) hosting an isolated bright single emitter (red spot). (b) The measured second order intensity-intensity correlation function (g (τ)) shows anti-bunching dip at τ=0, implying signature of single photon emission.

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Hi-End Cost-Effective Indigenous Instruments for 2-dim Materials Research

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Abstract

Results for the synthesis of graphene, MoS2, MOSe2 using a fully-automated indigenous Chemical Vapor Deposition System will be presented. Their characterization using an indigenous Variable Temperature STM and Physical Quantities Measurement System will be discussed. Some insights into the developmental aspects of the instruementation involved will be provided.

THURSDAY, 23 November, 2023		
Session 10A, GBR, Session Chair: Prasana Kumar Sahoo		
10A-1	09:00-09:30	**[Keynote] Michael Fuhrer** Two-Dimensional Topological Materials for Low-Voltage Transistors
10A-2	09:30-10:00	**[Invited] Anindya Das** Electric field tunable superconductivity in near magic-angle twisted bilayer graphene
10A-3	10:00-10:15	**[Contributed] Ipsita Das** Magnetic field driven states in magic-angle twisted bilayer graphene
10A-4	10:15-10:30	**[Contributed] Ayshi Mukherjee** Magic-angle twisted trilayer graphene: Inhomogeneous twisted superconductor showing competing magnetic order
Session 10B, Lalit 1-2, Session Chair: Manish Jain		
10B-1	09:00-09:30	**[Invited] Mikito Koshino** Topological moiré trilayers
10B-2	09:30-10:00	**[Invited] Ananth Govind Rajan** Computational Modeling of the Synthesis and Applications of Nanoporous 2D Materials
10B-3	10:00-10:15	**[Contributed] Sapta Sindhu Paul Chowdhury** Anomalous Phonon Thermal Transport in Germanene Monolayer
10B-4	10:15-10:30	**[Contributed] Shinjan Mandal** Electron-phonon interactions in twisted bilayer Graphene
Session 10C, Lalit 3-4, Focus session on Academia-Industry Translation, Session Chair: Arindam Ghosh		
10C-1	09:00-09:30	**[Invited] Barbaros Oezyilmaz** 2D Amorphous Materials and their Properties: From Ultra-Low k Dielectrics to Ferromagnetism in Co doped 2D NbSe2
10C-2	09:30-10:00	**[Invited] Aravind Vijayaraghavan** Graphene Technologies - from Lab to Market
10C-3	10:00-10:30	**NIL**
COFFEE BREAK, 10:30-11:00		
Session 11A, GBR, Session Chair: Aveek Bid		
11A-1	11:00-11:30	**[Keynote] Mandar M. Deshmukh** Superconducting van der Waals devices for quantum technology
11A-2	11:30-12:00	**[Invited] Ashish Arora**

		Magneto-optics of neutral and charged excitons in 2D materials: low fields versus high fields
11A-3	12:00-12:15	**[Contributed] Saisab Bhowmik** Valley polarized malleable bands near half filling in twisted bilayer graphene
11A-4	12:15-12:30	**[Contributed] Priya Tiwari** Experimental observation of spin−split energy dispersion in high-mobility single-layer graphene/WSe2 heterostructures
Session 11B, Lalit 1-2, Session Chair:Vishwanath Balakrishnan		
11B-1	11:00-11:30	**[Invited] Bharti Singh** Progress in PVDF and 2D Layered Materials based Nanocomposites for Energy Harvesting Applications
11B-2	11:30-11:45	**[Contributed] Rajeev Mehta** Evaluation of Nano-Reinforced Epoxy Coatings for Enhanced Corrosion Inhibition in Reinforcing Bars in Concrete Structures
11B-3	11:45-12:00	**[Contributed] Vidya Kochat** Raman spectroscopic studies of lattice dynamics and electronic structure evolution in twisted bilayer 2D materials
11B-4	12:00-12:15	**[Contributed] Siri Chandana Amarakonda** Augmenting the oxidation resistance of two-dimensional MXenes: A study on the role of antioxidants in aqueous dispersions
11B-5	12:15-12:30	**[Contributed] Aparna Rathi** Extremely large osmotic power with arrays of Angstrom scale capillaries of vermiculite
Session 11C, Lalit 3-4 , Session Chair: Sreedhara M B		
11C-1	11:00-11:30	**[Invited] Tomoki Machida** Symmetry engineering and subband electronics using van der Waals assembly of transition metal dichalcogenides
11C-2	11:30-12:00	**[Invited] Hongtao Yuan** Symmetry-Breaking-Induced Emergent Non-linear Phenomena at Van der Waals Heterostructures
11C-3	12:00-12:15	**[Contributed] A. Mohapatra** Tuneable thermal conductivity of multi-layer graphene: Role of turbostraticity and local curvature
11C-4	12:15-12:30	**[Contributed] Sonal Maheshwari** Cost effective route to produce Graphene from pet coke
LUNCH BREAK: 12:30-14:00		
Session 12A, GBR, Session Chair: Ageeth Bol		
12A-1	14:00-14:30	**[Invited] Kenneth S Burch**

		Detecting Emergent Quasi-particles in 2D Materials
12A-2	14:30-15:00	**[Invited] Tanuja Mohanty** Tuning of linear and non-linear optical properties of 2D semiconducting materials
12A-3	15:00-15:15	**[Contributed] Sudipta Majumder** Understanding the Origin of High Mobility in Mo Foil Grown Monolayer MoS2 Transistors
12A-4	15:15-15:30	**[Contributed] Sreedhara MB** Asymmetric “misfit” layered compounds: Chemical affinity outwits the entropy at high-temperature solid-state reactions
Session 12B, Lalit 1-2, NIL		
Session 12C, Lalit 3-4, Session Chair: Chandan Kumar		
12C-1	14:00-14:30	**[Invited] Viswanath Balakrishnan** Nanomanufacturing, Mechanical Reliability and Stability of 2D Materials
12C-2	14:30-15:00	**[Invited] Pramod Kumar Nayak** CVD synthesis of twisted 2D homo/hetero-bilayers for twistronics
12C-3	15:00-15:15	**[Contributed] Isha Atrey** Completely trilayer graphene dispersion provides film of high specific capacitance
12C-4	15:15-15:30	**[Contributed] Abdul Kaium Mia** Self-Powered Metal–Semiconductor–Metal 2D WS2 monolayer Photodetector with Asymmetric Contacts
COFFEE BREAK, 15:30-16:00		
CLOSING CEREMONY, 16:00-16:30, GBR		

Two-Dimensional Topological Materials for Low-Voltage Transistors

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The impending end of Moore's Law has prompted a search for a new computing technology with vastly lower energy consumed per operation than silicon CMOS. The recent discovery of topological phases of matter offers a possible solution: a "topological transistor" in which an electric field tunes a two-dimensional material from a conventional insulator "off" state to a topological insulator "on" state, in which topologically protected edge modes carry dissipationless current. This electric field-tuned topological transition has advantages over current MOSFETs: (1) Due to the combined effects of Rashba spin-orbit interaction and electric field control of the bandgap, the topological transistor may switch at lower voltage, overcoming "Boltzmann's tyranny"[1], and (2) true electric field-controlled switching opens the possibility of using the full power of negative capacitance structures as an electric field amplifier to achieve further reductions in switching voltage[2] (see Fig. 1). We have studied thin films of Na_3Bi grown in ultra-high vacuum by molecular beam epitaxy as a platform for topological electronic devices. When thinned to a few atomic layers Na_3Bi is a large gap (>300 meV) 2D topological insulator, and electrical transport measurements demonstrate that the current is carried by helical topological edge modes over millimeter-scale distances[3]. Electric field applied by proximity of an STM tip can close the bandgap completely and reopen it as a conventional insulator[4] demonstrating the basis of electric field-switched topology.

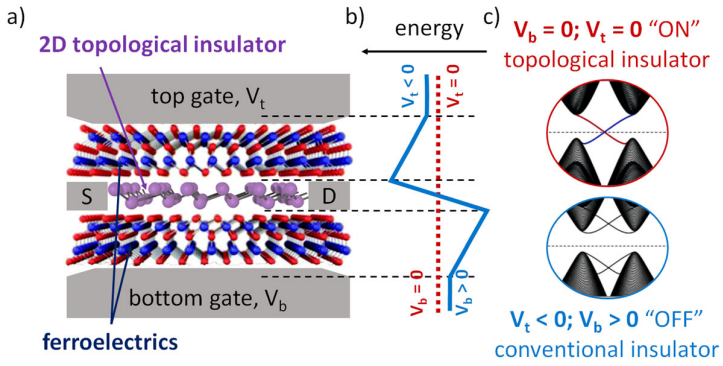

Figure 1. Schematic of negative capacitance topological quantum field-effect transistor. (a) Structure of the device. (b) Electrostatic potential energy as a function of distance across the device in "on" (red) and "off" (blue) states. (c) Band diagrams in "on" (topological insulator, red) and "off" (co nventional insulator, blue) states. After Ref. [2].

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Electric field tunable superconductivity in near magic-angle twisted bilayer graphene

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Superconductivity (SC) has been previously reported in magic-angle twisted bilayer graphene (MATBLG) with the variation of carrier concentrations, twist angles and the screening strength to shed insights into its origin, and shown no necessary concomitance between the SC and the correlation. Here we report the electric field tunable superconductivity in a near magic-angle twisted bilayer graphene with twist angle of 0.95◦. At zero displacement field (D), we observe the superconductivity at $\nu = 2.7$ around the van Hove singularities (vHS), which shifts to higher filling with the application of displacement field, and the optimal doping for the SC phase closely follows the vHS. At higher field (D>0.25 V/nm), the superconducting transition temperature (Tc) starts to diminish quite rapidly together with the prominent appearance of the Fermi surface resetting. The displacement field induced band structure and its role on SC in the present study has potential to shed light on the possible origin of SC in MATBLG.

Magnetic field driven states in magic-angle twisted bilayer graphene

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The recent discovery of magic angle twisted bilayer graphene (MATBG), in which two sheets of monolayer graphene are precisely stacked to a specific angle, has opened a plethora of new opportunities in the field of topology, superconductivity, and other strongly correlated effects. In twisted van der Waals materials, lattice mismatch can generate moiré patterns, which act as an additional periodicity that has a length scale order of magnitude larger than the underlying atomic lattice scale. For MATBG with a small twist angle close to θ=1.1°, the electronic bands are flattened by the periodic potential of the moiré bands and isolated from higher-energy dispersive bands. These flat electronic bands in MATBG have recently emerged as a rich platform to explore strong correlations. We report a rich sequence of wedge-like regions of quantized Hall conductance with Chern numbers C = ±1, ±2, ±3 and ±4, which nucleate from integer fillings of the moiré unit cell ν = ±3, ±2, ±1 and 0, respectively. The exact sequence and correspondence of the Chern numbers and filling factors suggest that these states are directly driven by electronic interactions, which specifically break the time-reversal symmetry in the system. The analysis of Landau-level crossings from higher energy bands enables a parameter-free comparison to a newly derived 'magic series' of level crossings in a magnetic field and provides constraints on the parameters of the Bistritzer–MacDonald MATBG Hamiltonian [1]. Additionally, we studied the detailed magnetotransport behaviour of the Hofstadter spectrum of MATBG. We observed the re-entrance of insulating states at ν = +2, ±3 of the moiré unit cell of MATBG upon applying an external magnetic field close to the full flux quantum Φ/Φ_0 = 1 of the superlattice unit cell (B = 25θ^2 T) and interaction-driven Fermi-surface reconstructions at other fillings, which are identified by new sets of Landau levels originating from these. These experimental observations are supplemented by theoretical work that predicts a new set of eight well-isolated flat bands at Φ_0, of comparable band width, but with different topology than in zero field [2].

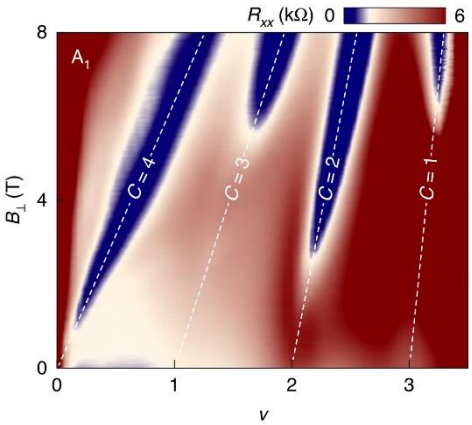

Figure 1. Color plot of R_{xx} as a function of B and ν showing the Chern insulators

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Magic-angle twisted trilayer graphene: Inhomogeneous twisted superconductor showing competing magnetic order

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Twisted graphene systems form an exciting platform to study the effects of strong electronic correlations arising due to flat bands. Members of the twisted graphene family like magic-angle twisted bilayer graphene and magic-angle twisted trilayer graphene (MATTG) exhibit superconductivity [1, 2]. The origin of this unconventional superconductivity largely remains elusive. In our experiments with the MATTG, we observe evidence of MATTG being an inhomogeneous superconductor due to the presence of moiré solitons and twistons [3]; creating weak links in the superconductor which behave like an array of Josephson junctions. We gather large statistics on the switching from the superconducting to the normal state - the switching distributions. These distributions are studied with the variation of temperature and in-plane magnetic field providing evidence of a competing magnetic order in the ground state. Also, our DC I-V characteristics, on analysis, reveal a broadened BKT transition as we extract the superfluid stiffness J_s~0.15 K in MATTG.

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Topological moiré trilayers

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In addition to the extensive study of twisted moiré bilayers in the past decade, the scope of investigation has extended to encompass multilayer systems including three or more layers. Particular attention has recently been directed toward twisted trilayer systems, which consist of three layers arranged in a specific rotational configuration. A twisted trilayer is characterized by two twist angles between adjacent layers, offering a vast parameter space that remains largely unexplored.

In the first part of my talk, we will present systematic theoretical studies on the lattice relaxation and the electronic structures in general twisted trilayer graphenes [1]. We show that the relaxed lattice structure forms a patchwork of moiré-of-moiré domains, where a moiré pattern given by layer 1 and 2 and another pattern given by layer 2 and 3 become locally commensurate. The electronic band calculation reveals a wide energy window featuring sparsely distributed highly one-dimensional electron bands. These one-dimensional states exhibit a sharp localization at the boundaries between supermoiré domains, and they are identified as a topological boundary state between distinct Chern insulators.

In the latter part of our discussion, we will explore the electronic structure of hBN / graphene / hBN trilayer system with arbitrary twist angles. We find that the electronic spectrum displays fractal minigaps akin to the Hofstadter butterfly. Each of minigaps is uniquely labeled by six topological numbers associated with the quasicrystalline Brillouin zones, and these numbers can be expressed as second Chern numbers through a formal connection with the quantum Hall effect in four-dimensional space [2,3].

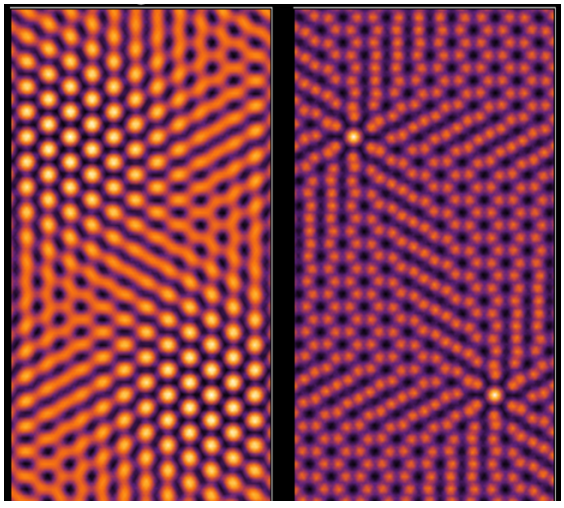

Figure 1. Moiré-of-moiré domain fomation in twisted tilayer graphene. The left and right panels illustrate the moiré pattern in the rigid and relaxed lattices, respectively.

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Computational Modeling of the Synthesis and Applications of Nanoporous 2D Materials

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Abstract

The controlled synthesis of two-dimensional (2D) materials and their nanoporous forms is a prominent challenge in nanotechnology. Chemical vapor deposition (CVD) is a scalable route to synthesize nanoporous 2D materials, including transition metal dichalcogenides (TMDs), for various applications. Nevertheless, the nucleation and growth of 2D TMDs during CVD and the formation of nanopores in them are not well understood. In this talk, I will discuss our group's recent work on using first-principles calculations within the framework of density functional theory (DFT) to understand the synthesis of 2D molybdenum disulfide (MoS_2) from metal-organic precursors. I will present an extensive set of DFT calculations that reveal the mechanism of MoS_2 formation during CVD by capturing previously unidentified elementary reactions. I will show the existence of thermodynamic and kinetic control over various edges present in a MoS_2 flake. Subsequently, I will discuss the application of a theoretical framework based on Marcus theory for atom-transfer reactions to understand the mechanism of nanopore formation in MoS_2. I will show that silicon single atoms play an important role in the nucleation of nanopores in MoS_2 under an electron beam. Next, I will outline the development of a machine learning model, supported by DFT calculations and kinetic Monte Carlo simulations, that can predict the formation time and probability of any arbitrary nanopore shape in graphene. Finally, I will discuss how nanoporous defects and grain boundaries in 2D materials can modulate water and ion transport on and through these materials. Overall, the multi-scale simulations presented in this talk will help understand and advance the synthesis and use of nanoporous 2D materials for various applications.

Anomalous Phonon Thermal Transport in Germanene Monolayer

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Thermal transport in germanene is intriguing yet challenging to investigate due to its buckled topology [1, 2]. Using the classical Stillinger-Weber potential, we have calculated the thermal conductivity of monolayer germanene under the framework of molecular dynamics simulations. We find an anomalous trend in the variation of thermal conductivity with temperature. Specifically, we observe a rapid decay of thermal conductivity till near room temperature, at which point the rate of decay slows down with temperature. To further our understanding, we investigate the variation of the thermal conductivity with the dimension of the monolayer sample using nonequilibrium molecular dynamics simulations. We notice that the thermal conductivity increases with the sample size, showing a diverging trend. We have conducted detailed phonon calculations with the phonon spectral energy density approach to understand this usual behavior. We will highlight our findings on this anomalous thermal transport in the monolayer germanene 2D system in this presentation.

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Electron-phonon interactions in twisted bilayer Graphene

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In twisted bilayer graphene, there is strong evidence that the electron phonon interactions mediate the transport properties [1, 2]. We have computed the electron phonon interactions in these systems as a function of twist angle and doping. The phonon modes are calculated using classical force fields and the electronic band structures are obtained using an atomistic tight-binding model with a Hartree potential built into the model [3]. The electron-phonon contribution to the phonon linewidth is calculated within the Migdal approximation.

In the first part of the talk, we provide estimates of the phonon linewidths that can be observed under experimental conditions in these systems and discuss the effects of electron phonon interactions on the phonon lifetimes. On top of the contribution to the phonon linewidth from the electron phonon interaction, we use mode projected velocity autocorrelation functions for calculating the phonon-phonon contribution to the phonon linewidths. This approach includes three, four and higher phonon-phonon interactions (up to all orders).

In the second part of the talk, we report our computations of the resistivity as a function of twist angle and doping and discuss the effects of the electron phonon interactions on the transport properties of this system. In our calculations we look at the scattering from all the phonon modes, instead of just the acoustic phonon modes considered in presently available studies.

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2D Amorphous Materials and their Properties:
From Ultra-Low k Dielectrics to Ferromagnetism in Co doped 2D NbSe2

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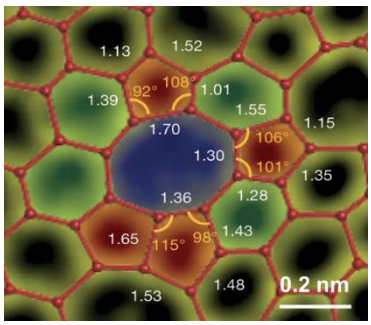

Disordered systems in the atomic limit offer several existing possibilities in both basic science and applications which are difficult to realize with 2D crystals. Examples range from higher order topological insulators to perfect Li ion membranes/solid state electrolytes. In my talk I will discuss two examples. First, I will discuss the synthesis, properties, and applications of monolayer amorphous carbon (MAC), the only realization of a free standing 2D amorphous material so far [1]. Extensive characterization by transmission electron microscopy reveals the complete absence of long-range periodicity and a threefold-coordinated structure with a wide distribution of bond lengths, bond angles, and five-, six-, seven- and eight-member rings. I will discuss its potential use as an atomically thin diffusion barrier and as an ultra-low k dielectric. Combined with its low-temperature synthesis by laser-CVD, these are critical features to enable substantial improvements in silicon-based semiconductor electronics and ensure compatibility with future 2D electronics. For energy applications, e.g., as supercapacitors such materials can also be synthesised as nano-porous monolithic amorphous carbon foam using spark plasma sintering (SPS).

Next, I will discuss the role of disorder in atomically thin niobium diselenide ($NbSe_2$) intercalated with dilute cobalt (Co) atoms and show that such systems spontaneously display ferromagnetism below the superconducting transition temperature (T_C). We elucidate the origin of this phase by constructing a magnetic tunnel junction that consists of Co and Co doped $NbSe_2$ as the two ferromagnetic electrodes. At a temperature well below T_C, the tunnelling magnetoresistance shows a bistable state, suggesting a ferromagnetic order in superconducting Co-$NbSe_2$ [2]. We propose a RKKY exchange coupling mechanism based on spin-triplet superconducting order parameter to mediate such ferromagnetism. Non-local lateral spin valve measurements with Hanle spin precession signals up to micrometres below T_C suggest an intrinsic spin-triplet state in superconducting $NbSe_2$ as key ingredient.

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Graphene Technologies – From Lab to Market

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Graphene was first isolated at the University of Manchester in 2004. Since then, significant strides have been made in studying and understanding the fundamental properties of Graphene and other 2D Materials. Before long, the potential for graphene in real world applications in a range of products across all sectors became apparent. The University of Manchester established the National Graphene Institute and the Graphene Engineering Innovation Centre to bridge the gap between academia and industry, in order to accelerate the commercialization of graphene based technologies and products.

In this talk, I will summarize my efforts at Manchester to bring graphene technologies developed in my lab to market through a number of case studies. The most successful example of this is in the area of composites. My group works extensively on the development of graphene enhanced elastomers and foams for improvements in structural and electronic properties. We have partnered with a British International footwear brand Inov-8 Ltd to bring graphene enhanced rubber outsoles and foam midsoles to the global market in Inov-8 high-performance sports shoes. The graphene enhanced rubber delivers high grip and high durability outsoles while the foam delivers high and long-lasting energy return for midsoles. This technology is further being developed and commercialized through a spin-out company called Grafine Ltd.

In the area of sensors, we have developed graphene based capacitive force and touch sensors, implemented both on rigid silicon-based MEMS platform and transparent and flexible platforms. We have stablished a spin-out company, Atomic Mechanics Ltd, which has developed a graphene based transparent and flexible touch sensor for human machine interface applications such as robotics. I will also present some of the other technologies being developed in my lab that have significant commercial potential in forthcoming years.

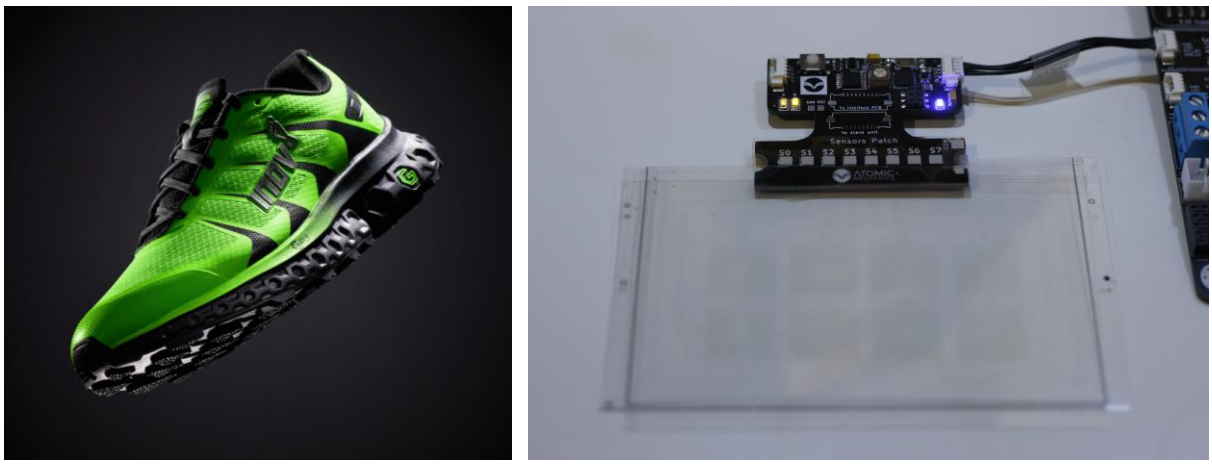

Figure 1. Graphene products and prototypes. (a) Inov-8 Graphene Shoe. (b) Atomic Mechanics Graphene touch sensor array.

Superconducting van der Waals devices for quantum technology

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2D van der Waals materials-based heterostructures have led to new devices for fundamental science and applications. Superconducting devices based on 2D materials offer unique opportunities to engineer new functionality. I will present results from two classes of materials. First, proximitized graphene-based Josephson junctions lead to a quantum noise-limited parametric amplifier with performance comparable to best discrete amplifiers in this class [1]. Gate tunability of the center frequency of the amplifier, rather than flux, offers key advantages. An extension of graphene Josephson architecture is to make state-of-the-art bolometers, leveraging graphene's low specific heat, and I will present initial results. Second, twisted van der Waals heterostructures based on high Tc superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ lead to the realization of a high-temperature Josephson diode [2]. Such Josephson diodes offer an opportunity to engineer the current phase relationship and the resulting inductive response for many applications close to liquid nitrogen temperature.

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Speaker: Ashish Arora, IISER Pune

Title: Magneto-optics of neutral and charged excitons in 2D materials: low fields versus high fields

Abstract. Magneto-optical spectroscopy methods such as magneto photoluminescence, magneto absorption, Faraday effect, and magneto-optical Kerr effect are powerful tools to investigate the spin-valley-layer physics of 2D materials. They are vital to many discoveries such as valley Zeeman effect, magneto-field-induced valley polarization, single-photon emitters, interlayer and intralayer excitons, Landau quantization of a 2D electron/hole gas and moiré excitons in 2D semiconductors and their heterostructures [1]. In near future, they are expected to play a central role in a new generation of energy efficient spin-valley-based devices.

In this talk, I will describe some of our high-field (up to 30 T) magneto-optical spectroscopy investigations of neutral and charged excitons in 2D materials such as interlayer excitons, valley polarization of trions, magnetic control of exciton intervalley phase, and layer dependent valley Zeeman effects [1]. However, since such large magnetic fields are not readily available to the users, I will describe our newly invented Faraday rotation spectroscopy method, which enables sensitive spectroscopy under small magnetic fields such as 1T with large spectral acquisition speeds [2]. The new technique enables measuring Valley Zeeman effects such as Zeeman splitting and valley polarization on 2D semiconductors, as well as fast hysteresis loop measurements on 2D magnets with high precision [2]. I will also present our recent discovery of excited-state 2s trions in a GaAs quantum well using MOKE spectroscopy under magnetic fields up to 7 T [3], drawing parallels with their recent discovery in a 2D material [4].

Our work paves the way for new discoveries using high-precision magneto-optical spectroscopy of 2D semiconductors, magnets and their heterostructures with high efficiency.

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Valley polarized malleable bands near half filling in twisted bilayer graphene

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When two layers of graphene are rotated at the magic angle, the low-energy electronic bands become exceptionally narrow due to strong interlayer hybridization. Flat bands provide an ideal platform for exploring strongly correlated physics that cannot be explained by single-particle calculations. In recent years, magic angle twisted bilayer graphene (MATBG) has demonstrated its potential to host a diverse range of correlated phases, including correlated insulators, superconductivity, orbital ferromagnetism, strange metal behavior, Chern insulators, density waves, and nematicity. Interestingly, these phases are highly tunable through external perturbations such as electromagnetic fields, temperature, pressure, and dielectric environments. In this study, we have performed magnetotransport measurements in MATBG proximitized by a layer of tungsten diselenide (WSe_2), inducing a finite spin-orbit coupling in the system. We find anomalous Hall effect near the half filling ($\nu = 2$) with an abrupt switching of magnetization, which can be controlled by the carrier density in the system. A series of Lifshitz transitions accompany the hysteresis near $\nu = 2$ in the zero magnetic field limit. As the magnetic field is increased, we observe the emergence of a perfectly quantized Chern insulator state at $\nu = 2$. The main findings of our work point towards the existence of valley-polarized ground states in the vicinity of $\nu = 2$, which are stabilized by the presence of spin-orbit coupling.

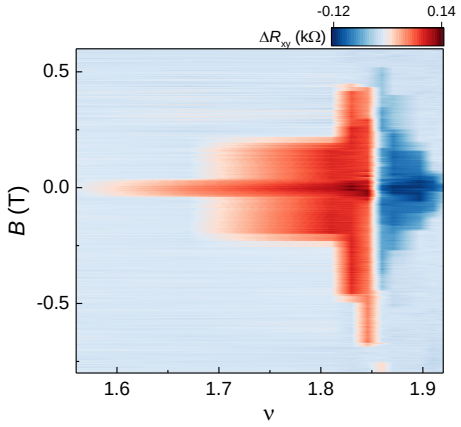

Figure. Switching of magnetization near $\nu = 2$. The difference between the values of Hall resistance for the opposite magnetic field sweeps plotted as a function of the magnetic field B and filling fraction ν. The change in colour from red to blue at $\nu = 1.85$ indicates the reversal of magnetization.

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Experimental observation of spin−split energy dispersion in high-mobility single-layer graphene/WSe2 heterostructures

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Proximity-induced spin–orbit coupling in graphene has led to the observation of intriguing phenomena like time-reversal invariant Z2 topological phase and spin-orbital filtering effects. An understanding of the effect of spin–orbit coupling on the band structure of graphene is essential if these exciting observations are to be transformed into real-world applications. In this research article, we report the experimental determination of the band structure of single-layer graphene (SLG) in the presence of strong proximity induced spin–orbit coupling. We achieve this in high-mobility hexagonal boron nitride (hBN)-encapsulated SLG/WSe_2 heterostructures through measurements of quantum oscillations. We observe clear spin-splitting of the graphene bands along with a substantial increase in the Fermi velocity. Using a theoretical model with realistic parameters to fit our experimental data, we uncover evidence of a band gap opening and band inversion in the SLG. Further, we establish that the deviation of the low-energy band structure from pristine SLG is determined primarily by the valley-Zeeman SOC and Rashba SOC, with the Kane–Mele SOC being inconsequential. Despite robust theoretical predictions and observations of band-splitting, a quantitative measure of the spin-splitting of the valence and the conduction bands and the consequent low-energy dispersion relation in SLG was missing—our combined experimental and theoretical study fills this lacuna.

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P. Tiwari et al. npj 2D Materials and Applications 6, 68 (2022)

Progress in PVDF and 2D Layered Materials based Nanocomposites for Energy Harvesting Applications

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Abstract:- As the world enters into the era of IoT, artificial intelligence, and 5G technology era, there is an upsurge thrust in smart, miniaturized, flexible electronic devices. Until now, the energy need of these devices are fulfilled by traditional batteries and energy storage devices. A suitable alternative to this is to harvest energy from the surrounding environment. Among various energy harvesting technologies, harvesting the micro-nano mechanical energy with the help of piezoelectric and triboelectric nanogenerators is a potential solution to fulfill the requirements of booming sustainable energy in the new era which can convert irregular mechanical energy to electrical energy. Poly(vinylidene fluoride) PVDF is the most explored piezoelectric semicrystalline polymer material which is known for their excellent flexibility, biocompatibility, low cost, and ease of processing[1]. 2D materials possessing numerous remarkable properties including high electrical conductivity, mechanical strength, optical transparency, and most importantly superior intrinsic piezoelectric properties have been the center of discussion and hence therefore can be combined with PVDF to design flexible piezoelectric and triboelectric nanogenerator[2]. Our group is working on enhancing the output performance of the PVDF-based nanogenerator by doping it with various 2D materials such as rGO, MoS_2, $MoSe_2$, and so on as nanofillers materials, which have potential applications in powering electronic devices to design self-powered devices, water splitting technique, dye degradation, and so on.

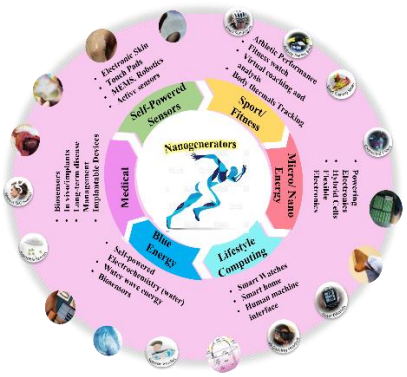

Figure 1. Potential application areas of the piezoelectric and triboelectric nanogenerator

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Evaluation of Nano-Reinforced Epoxy Coatings for Enhanced Corrosion Inhibition in Reinforcing Bars in Concrete Structures

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Abstract

The corrosion of concrete infrastructures poses a significant challenge in the construction industry, requiring substantial financial investment for repair and rehabilitation worldwide. Among the effective methods to mitigate steel corrosion, epoxy coatings on reinforcing bars have shown promising results. In our work, we focus on enhancing the corrosion resistance of epoxy coatings by incorporating a hybrid of graphene derivatives and carbon nanotubes (CNT), nano-clay, and self-healing tung-oil microcapsules. We subjected the coated samples to accelerated impressed current corrosion tests and evaluated their performance. To assess the effectiveness of the prepared epoxy coated samples, we employed non-destructive monitoring techniques including visual inspection, impressed corrosion current measurement, and ultrasonic guided wave measurement. The reliability of the non-destructive testing methods was further confirmed by conducting destructive testing, which involved measuring the mass loss and residual tensile strength of the corroded bars.

The incorporation of nano-reinforcements in epoxy coatings has proven to be highly effective in mitigating corrosion. Among the various coatings tested, the GO/CNT (Graphene Oxide/Carbon Nanotube) based coatings demonstrated superior performance, with no signs of corrosion initiation even after 150+ days of accelerated corrosion testing. Comparatively, the GO and rGO (reduced Graphene Oxide) based coatings outperformed the nano-clay based coatings. Furthermore, the tung-oil microcapsules-based coatings, known for their self-healing properties, successfully arrested corrosion after its initiation, as confirmed by non-destructive testing methods. This study showcases the significant corrosion inhibition achieved through the use of modified epoxy coatings. It represents an important step towards sustainable construction practices that require less frequent repair and rehabilitation, thereby contributing to the goal of achieving sustainable construction.

Keywords: Corrosion, epoxy coatings, ultrasonic guided waves, corrosion current, graphene oxide, reduced graphene oxide, carbon nano-tubes, nano-clays, and tung-oil microcapsules

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Raman spectroscopic studies of lattice dynamics and electronic structure evolution in twisted bilayer 2D materials

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ABSTRACT

The 2D layered materials or the van der Waals materials comprise a new class of quantum materials, offering pioneering advances in fields of nanoelectronics, photonics and spintronics. The abundance of 2D materials identified and isolated in the last decade along with their numerous combinations translating to 2D heterostructures with varied functionalities has accelerated the research in these novel materials towards development of nanoscale devices with emergent and unique properties. Contrary to many other materials, the 2D materials also have another fascinating degree of freedom in terms of controlling the twist angle between the adjacent layers thereby modulating the mechanical and electronic coupling between the layers which has resulted in several emergent phases such as correlated insulator states, superconductivity, quantum criticality and Moiré excitons. In this work, we explore the evolution of Moiré periodic potential by tuning the twist angle and its influence on the mechanical and electronic coupling between the layers in 2D bilayer systems of graphene and transition metal dichalcogenides (TMDs). The various scattering processes and resonance mechanisms in twisted bilayer systems have been investigated using the spectroscopic techniques of Raman and photoluminescence. Another interesting aspect of the 2D TMDs is their preferential stacking configurations which are also associated with distinct electronic behaviour. We also discuss about the identification of various stacking configurations of 2D TMDs using resonance Raman spectroscopy which is particularly useful in the growth of large area bilayer TMDs. In twisted bilayer graphene (TBLG) superlattices, we observe that the electron-phonon scattering is dependent on the electronic structure which evolves as a function of the twist angle between the graphene layers and the Moiré potential. The Raman signatures of the combination modes also reveal a commensurate – incommensurate transition in TBLG at large twist angles.

KEYWORDS
Twisted bilayer graphene, twisted bilayer transition metal chalcogenides, Raman spectroscopy, Moiré potential, stacking configuration

Augmenting the oxidation resistance of two-dimensional MXenes: A study on the role of antioxidants in aqueous dispersions

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Two-Dimensional (2D) $Ti_3C_2T_x$, belonging to a family of MXenes, have attracted tremendous interest in the scientific community because of their myriad applications in energy storage and conversion, EMI shielding, and sensors. The major drawback of these MXenes is their susceptibility to oxidation when stored in water under ambient conditions. Several techniques have been explored to arrest the oxidation of MXenes, such as storage at extremely low temperatures (-18 and -80 °C), but these prove to be energy-intensive processes[1]. Storage in organic solvents mitigates oxidation, but the dispersion stability of MXenes is poor in these solvents. Storing in Sodium Ascorbate, an antioxidant, has proven to be an effective solution to enhance the oxidation resistance of MXenes[2]. However, very little is understood about the interaction mechanism of MXenes and antioxidants and also the choice of antioxidants. Herein, we explore the role of various antioxidants, majorly used in the food and pharmaceutical industry, on the oxidation stability of MXenes. While some antioxidants accelerate oxidation, some do not show any effect, and some antioxidants have proven successful in storing MXene for up to 60 days. The performance of these antioxidants further enhances when two of them are combined, indicating a synergistic effect, a strategy we also employ in our study of MXene's chemical stability. This paper explores the interactions between antioxidants and MXenes when stored at different pH levels and temperatures. We have further explored the potential applications of these antioxidant-protected MXenes in energy storage devices, such as microsupercapacitors. Even after 30 days of fabrication of the screen-printed microsupercapacitors with antioxidant-protected MXene, these exhibit an areal capacitance fairly identical to day 1 when kept in ambient conditions without an encapsulation. This study provides a potential solution to an ever-lasting problem in the field of MXenes.

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Extremely large osmotic power with arrays of Angstrom scale capillaries of vermiculite

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In the domain of osmotic power generation, attaining a requisite power density of 5 W/m² has been challenging due to the intricate demand for capillaries proximal in scale to that of ions and molecules. In this study, we successfully fabricated water-stable and precisely controlled membranes composed of sodium-vermiculite, exhibiting a capillary size of ~ 5 Å. Interestingly, these membranes exhibit an exceptional cation selectivity of 0.83, coupled with an impressive conductivity, resulting in a substantial power density of 9.6 W/m^2 when subjected to NaCl concentration gradients of 50 at a temperature of 296 K. Remarkably, the power density shows a tremendous increase with temperature, reaching an extremely large value of 65.1 W/m^2 for a concentration gradient of 50 at 333 K, the highest ever reported. This markedly differs from the classical behavior and indicates the role of ion (de)hydration in enhancing power density. Our work opens new possibilities for exploiting (de)hydration-based membrane devices for energy harvesting applications.

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Symmetry engineering and subband electronics using van der Waals assembly of transition metal dichalcogenides

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We demonstrate that the spatial inversion symmetry and hence the spin splitting in band structure can be controlled by van der Waals (vdW) assembly with a controlled twist angle. Twisted bilayer WTe_2 with twist angle θ_{twist} = 0° and 180° are investigated. The intensity of second harmonic generation changes by two orders of magnitude depending on θ_{twist}, indicating that 1L WTe_2 +1L WTe_2 (0°) possesses the spatial inversion symmetry, whereas 1L WTe_2 +1L WTe_2 (180°) lacks the inversion symmetry. The electronic structure of the 1L WTe_2 +1L WTe_2 are significantly modulated by θ_{twist}. The spin splitting emerges when θ_{twist} = 180° as a consequence of the broken inversion symmetry. The effect induced by controlling the symmetry is quite robust with respect to θ_{twist} fluctuation and inhomogeneity, suggesting the feasibility of pursuing new physical phenomena in 2D materials based on symmetry engineering.

Few-layer transition metal dichalcogenides (TMDs) exhibit subband quantization induced by the out-of-plane quantum confinement of the wavefunctions, i.e., a few-layer TMDs are naturally-formed quantum wells (QWs). Using momentum-conserved resonant tunneling, we investigate the QW states in 3L-WSe_2/h-BN/3L-WSe_2 van der Waals (vdW) tunnel junctions with twist angles θ_{tunnel}. Current–voltage characteristics exhibit multiple resonant tunneling peaks whose positions shift as θ_{tunnel} was varied over the 0–60° range. These results were in good agreement with calculated angular dispersion in conduction band in 3L-WSe_2, which indicated the presence of a spin-polarized subband crossing and a saddle point. Our twist-controlled resonant tunneling approach overcomes the difficulties associated with momentum-resolved electronic structure measurements and reveals the unique vdW-QW states in the conduction band of multi-layer WSe_2.

Finally, we demonstrate 3D manipulation of 2D material flakes, such as sliding, rotating, and folding. A PVC/PDMS micro-dome structure functions as a point-of-contact manipulator for 2D material flakes. The adhesion between the PVC polymer and 2D material is fully tunable with temperature. Our method could facilitate the expansion of van der Waals heterostructure fabrication technology for constructing more complex vdW structures.

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Symmetry-Breaking-Induced Emergent Non-linear Phenomena at Van der Waals Heterostructures

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Symmetry breaking in low-dimensional heterostructures can provide unprecedented possibilities to generate emergent quantum phenomena in condensed matter physics. Since lattice symmetry breaking at the heterointerfaces can produce the geometric deformation of energy dispersion due to the interfacial hybridization of atomic orbitals, the symmetry-mismatched van der Waals (vdW) heterointerface, beyond the individual quantum material, can serve as an excellent platform for realizing emergent non-linear phenomena. For example, the symmetry group of the WSe_2/BP heterointerface is the common sub-symmetry group of the crystalline symmetries in monolayer WSe_2 (C_{3v} rotational symmetry) and the BP thin flake (C_{2v} rotational symmetry), and thus the heterointerface will have no rotational symmetry (C_1 symmetry and no mirror symmetry for a generic twist angle). Therefore, the symmetry breaking at atomically-sharp vdW interfaces exhibits remarkable capabilities to control emergent electronic states and exotic quantum phenomena by forming moiré patterns with a specific lattice mismatch. However, experimental study with such a strategy remains elusive.

Here, we demonstrate, with a universal strategy to break lattice symmetry in stacked Van der Waals heterostructures, experimental observations of emergent nonlinear optical/transport phenomena including the spontaneous quantum mechanical shift current and the circular photogalvanic effect. Three examples are included here: 1) Although the rotational symmetry of each material prohibits the generation of such a shift current and spin photocurrent under normal incidence of light, we observe a direction-selective photocurrent response at the symmetry-mismatched heterointerface with a twist angle of 0° (mirror symmetry maintained), in which the shift current is found parallel to the mirror direction therein while the spin photocurrent is found perpendicular to the mirror. 2) Since such direction-selective nature corresponds to the direction of in-plane polarization and the Berry curvature dipole therein, we reveal that the spontaneous quantum mechanical shift current is associated with the topological electronic nature with in-plane polarization at the WSe_2/BP interface, while the circular photogalvanic effect originates from the inter-band Berry curvature dipole mechanism at a WSe_2/SiP interface. 3) We demonstrate that the bottom material with C_2 rotational symmetry not only produces symmetry breaking at interfaces but also behaves as an excellent dielectric material for gating. Note that giant anisotropy in both the optical response and electronic transport is found in TMDC/SiP_2 heterostructures. We realize a high-performance SiP_2-gated MoS_2 transistor with large on/off ratios > 10^5 and low leakage currents (far below the low power limit) and further observe an insulator-to-metal transition therein, indicating the great dielectric capability of the SiP_2 material. In short, we provide a new strategy for generating exotic functionalities and geometric features at twisted dielectric/semiconductor interfaces via symmetry engineering.

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Tuneable thermal conductivity of multi-layer graphene: Role of turbostraticity and local curvature

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The presence of rotational stacking faults and mechanical instabilities in two-dimensional systems has added a whole new dimension to the engineering of its physical properties. Turbostratic multilayer graphene belongs to the family of twisted graphene systems. It contains a distribution of rotational stacking faults, and the interfaces in this system also have variable twist angles. These twist angles can be obtained using the position of the R-modes in the Raman spectrum, together with its laser dependence. We have studied the influence of turbostratic single-layer graphene content on the thermal conductivity of a defect free multilayer graphene system. Thermal transport in these systems is investigated with Raman optothermal technique supported with finite element analysis simulations. Thermal conductivity of AB-stacked graphene diminishes by a factor of 2.59 for 1% of turbostratic single-layer graphene content, while the decrease at 19% turbostratic content is by an order in magnitude. Thermal conductivity obeys the relation, $\kappa \sim \exp(-F)$, where F is the fraction of turbostratic single-layer graphene content in the system. Mechanical instabilities such as wrinkles have been shown to have decreased the thermal conductivity of single layer graphene. In this case, an interesting local enhancement of thermal conductivity across wrinkles is observed, which is discussed in detail.

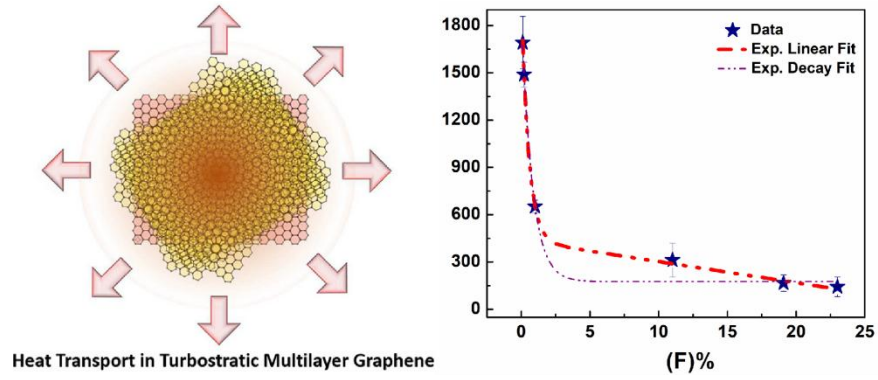

Figure 1. Schematic showing heat transport in turbostratic multilayer graphene and a large reduction in thermal conductivity with increase in turbostratic single layer graphene content (F)%.

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Title: Cost effective route to produce Graphene from pet coke

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Graphene is a single atomic layer carbon atoms organized in systematic honeycomb lattice having 2-3nm size. Due to its exceptional characteristics like mechanical strength, high electrical conductivity, chemical stability and high surface area, it has got applications in the area super capacitor, Li-ion Batteries inks and paints, sensors, solar cells and biological applications. The global graphene market is projected to reach $876.8 million by 2027, growing at a CAGR% of 40.2% from 2020 to 2027. The commercial price of graphene ranges from ₹ 15,000 to ₹ 25,000 per kg depending upon its purity and number of layers, however producing graphene at commercial scale is still a challenging job.

In the current study pet coke has been chosen a raw material for converting it to graphene via high temperature calcination and mechanical exfoliation. Product obtained was analyzed for its critical properties like Raman Spectra, surface area, no. of layers for its suitability for various applications. Further electrochemical studies like GCD, CVM and EIS were conducted on prepared product, and it was found that the product is showing good potential for super capacitor and battery charge storage applications. As pet coke in refinery is a low value product (Rs. 7-10 / Kg) and has got limited usage, production of graphene from pet coke will help refinery in improving GRM and will also give market a cost-effective product in upcoming energy storage devices. As Graphene is foreseen as breakthrough material of 21st century, the current route opted is easy to scale-up and will provide feasible solution for Graphene production on commercial scale.

Detecting Emergent Quasi-particles in 2D Materials

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Two-dimensional materials offer a plethora of novel phenomena, often revealed through new quasi-particles. States that emerge from combining quantum geometry and strong correlations are particularly interesting. Here I will discuss our group's efforts to detect the unique signatures of such quasi-particles using various spectroscopic tools. This is based on our advances in moving all fabrication and sample preparation into our cleanroom in a glovebox (Fig. 1).[2] I will focus on our recent discovery of the Axial Higgs mode from a Charge Density Wave and relativistic states in the 2D Rare-Earth Tritellurides.[1] Time permitting, I will also explain our efforts to reveal topological edge modes in exfoliated FeTeSe superconductors.[3]

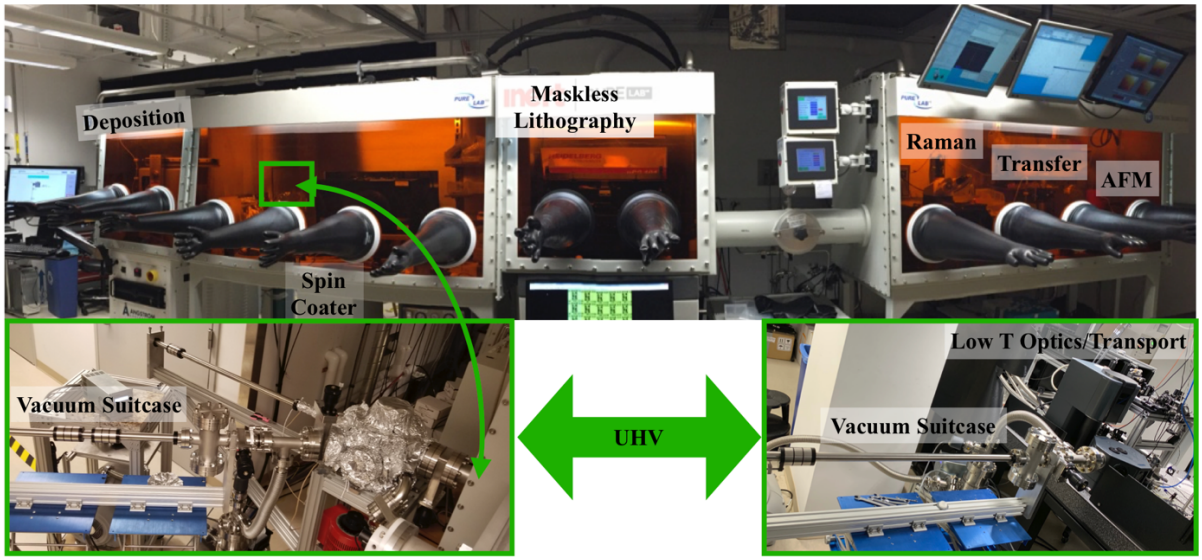

Figure 1. Cleanroom in a glovebox with fabrication and characterization. Ability to transfer via vacuum suitcase, in UHV, to/from low T optics/electronics and MBE(not shown).

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Tuning of linear and non-linear optical properties of 2D semiconducting materials

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Abstract

Development of 2D photonic materials possessing modulated linear and non-linear optical response find immense applications in optoelectronics. Our research work presents tuning of linear and nonlinear optical absorption in hBN with compositional variation both in heterostructure and nanocomposite form. Integration of graphene with hBN results in ternary boron carbon nitride (BCN) which has extraordinary attributes with respect to the graphene and hBN. Experimental and theoretical results indicate that the ternary BCN has the capability of bandgap modulation between graphene and hBN, from zero bandgap to broad bandgap (~6 eV) insulator. Moreover, the nonlinear optical absorption and nonlinear refractive index enhance due to the diffusive π electron access, bandgap narrowing and defect sites. Similarly, in GO-hBN nanocomposite, bandgap modulation with composition ratio indicates the introduction of intermediate states and charge transfer between these two domains consequently affecting the non-linear optical response. The nanocomposite with equal amount of GO and hBN exhibits minimum bandgap and enhanced non-linear properties.

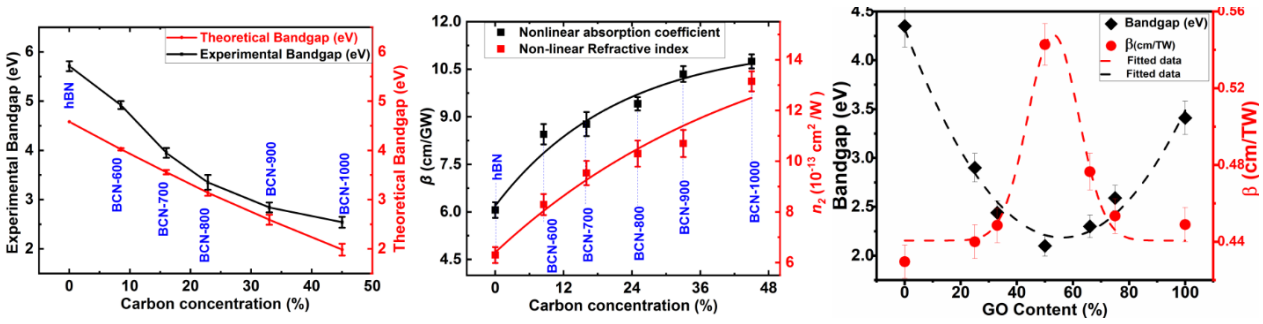

Fig. (a) Theoretical and experimental bandgap of BCN for varying carbon concentration. (b) nonlinear absorption coefficient and refractive index for BCN samples. (c) bandgap and nonlinear absorption coefficient for GO-hBN nanocomposite in different composition.

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Understanding the Origin of High Mobility in Mo Foil Grown Monolayer MoS_2 Transistors

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2D transition metal dichalcogenides (2D-TMDs) have gained significant interest as a novel category of materials due to their exceptional fundamental properties and applications in optoelectronic and nanoelectronic devices. In particular, Molybdenum Disulfide (MoS_2) has been extensively researched for its direct band gap, strong spin-orbit coupling, and high young's modulus in the monolayer limit. Therefore, there is a high demand for large-area synthesis of MoS_2 with good electrical transport properties. In this study, we have demonstrated a facile chemical vapour deposition (CVD) process for growing high mobility monolayer MoS_2 by a face to face metal precursor supply route (Figure 1). Plasma oxidized Molybdenum Foil (Mo Foil) was used as a metal precursor instead of Molybdenum Oxide (MoO_3) powder. The thin oxide layer on the foil provided consistent source of precursors across a wide range of temperatures and growth times. The MoS_2 samples were thoroughly characterized using Raman, photoluminescence (PL) spectroscopy, and transmission electron microscopy (TEM) revealing high quality of the as-grown samples. The resulting MoS_2 2D field-effect transistors (2D-FETs) exhibited high mobility, with the top-performing device achieving mobility exceeding 100 $cm^2V^{-1}s^{-1}$. Additionally, through low-temperature electrical transport studies we discovered that the presence of donor states likely caused by Sulphur vacancies near the conduction band is responsible for the increased conductivity in the FET channel through doping.

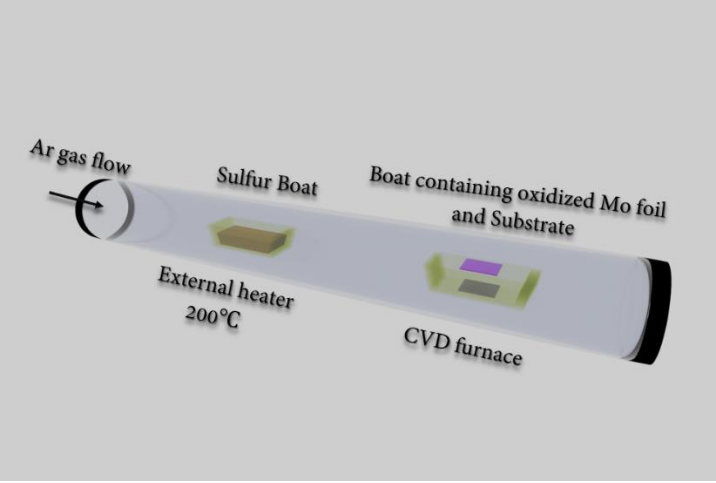

Figure 1. Schematic diagram of the CVD furnace containing the precursor boats in a face to face metal precursor supply route.

Asymmetric “misfit” layered compounds: Chemical affinity outwits the entropy at high-temperature solid-state reactions

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Abstract

Asymmetric two-dimensional (2D) structures (often named Janus), like SeMoS and their nanotubes, have tremendous scope in material chemistry, nanophotonics, and nanoelectronics due to a lack of inversion symmetry and time-reversal symmetry. The synthesis of these structures is fundamentally difficult owing to the entropy-driven randomized distribution of chalcogens. Indeed, no Janus nanotubes were experimentally prepared, so far. Serendipitously, a family of asymmetric misfit layer superstructures (tubes and flakes), including LaX-TaX_2 (where X = S/Se), were synthesized by high-temperature chemical vapor transport reaction in which the Se binds exclusively to the Ta atoms and La binds to S atoms rather than the anticipated random distribution. With increasing Se concentration, the LaS-TaX_2 misfit structure gradually transformed into a new LaS-$TaSe_2$-$TaSe_2$ superstructure. No misfit structures were found for X_{Se} =1. These counterintuitive results shed light on the chemical selectivity and stability of misfit compounds and 2D alloys, in general. The lack of inversion symmetry in these asymmetric compounds induces very large local electrical dipoles. The loss of inversion and time-reversal symmetries in the chiral nanotubes offers intriguing physical observations and applications.

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Nanomanufacturing, Mechanical Reliability and Stability of 2D Materials

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It is relatively easier to grow 2D materials by chemical vapor deposition and show measurable properties in small quantities while large scale manufacturing of 2D materials remains a bottleneck in realizing a variety of device applications. Scalable synthesis of 2D materials is not a linear journey and intertwined with the complex issues of quality, mechanical reliability, stability and performance. Lowering the cost of such system development based on 2D materials to an affordable price is another big challenge. We address few of the fundamental issues involved in large scale nanomanufacturing, mechanical reliability and stability of 2D materials that are very attractive for electrical, optical, environmental and energy applications. Generally, defects are produced during the CVD growth of 2D materials and post growth processes like transfer of flakes, and other processing steps result in fracture. We address the issue of microcracks and fractures in WS_2 by thermal stress engineering and post-growth atomic stitching strategies. The broken 2D material can be stitched by the same or different material, stitching with a different material giving rise to the formation of 2D heterostructure with enhanced optical emission at the interface. Recently, growth of 2D material on sapphire substrate gained interest among researchers to produce large area, crack free monolayers. Our nanoscratch investigation revealed low interfacial adhesion energy that promotes the easy delamination of monolayer grown on sapphire unlike the same grown on SiO_2 which shows higher adhesion and at the same time produces severe cracking in the case of WS_2 monolayer. Further, AFM experiments were carried out to investigate the friction and wear of the freshly grown WS_2 monolayer as well as aged WS_2 monolayer. We also probe chemical stability of CVD grown WS_2, MoS_2, $MoTe_2$ and mitigate their degradation kinetics by passivation as well as polymer encapsulation by composite approach. In addition to controlled CVD growth, several approaches such as electron beam patterning, direct writing by ballpoint pen, and fabrication of 2D materials based layered composites will be presented. For example, we demonstrate direct pen writing with a few layer MoS_2 in complex patterns that enables easy, affordable, and simple fabrication of energy storage devices towards distributed manufacturing and sustainability. Similarly, site-specific patterning of carbon nanostructures over atomically thin WS_2 monolayer has been achieved via direct electron beam induced deposition for data encryption by modulating the optical emission of the WS_2. Overall, large area growth and nano-engineering of 2D materials with uniform coverage, patterning, defects, issues of cracking, friction, wear and future prospects for improvements to ensure the reliability of 2D materials and low cost fabrication will be discussed.

CVD synthesis of twisted 2D homo/hetero-bilayers for twistronics

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Twistronics refers to the study of the electronic properties of materials that have been twisted or rotated with respect to each other. This term was first introduced in a bilayer graphene [1], where two layers of graphene were twisted at a specific angle, creating a moiré pattern that affected the electronic properties of the material. This effect has since been observed in other two-dimensional (2D) materials such as transition metal dichalcogenides (TMDs) and hexagonal boron nitride (h-BN). The ability to tune the electronic properties of materials through twistronics has numerous potential applications including development of novel electronic devices, such as transistors and sensors, optoelectronics, energy storage and so on. However, the major challenge for twistronics is the controlled synthesis of preferred twist angles for commensurate 2D lattices.

In this talk, I will cover the synthesis of twisted homobilayer and heterobilayer TMD systems using chemical vapor deposition (CVD) for twistronics. I will describe how a simple twist can dramatically changes the functionalities of twisted bilayer TMDs such as $MoSe_2/WSe_2$[2], $MoSe_2/WS_2$[3], and 2L WSe_2[4] thereby creating rich physics including the emergence of higher-order excitations such as trion, biexciton, interlayer exciton, hybrid exciton, moiré exciton and so on, which can give an insight into the physics of the many-body dynamics. Moreover, the thermal transport of a twisted bilayer (t-BL) is affected by the rotation of the atomic planes to the increased number of phonons scattering sites due to the incorporation of moiré superlattice. I will report the variation of thermal conductivity of CVD grown t-BL $MoSe_2$ using the optothermal Raman technique for selected twist angles [5]. Finally, I will summarize the current challenges and future opportunities in the field of twistronics.

References

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Completely trilayer graphene dispersion provides film of high specific capacitance

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Graphene has emerged as a remarkable material with diverse applications in the field of optoelectronics and energy storage. However, the challenge lies in producing high-quality graphene via liquid phase methods that can match the optoelectronic properties achieved through techniques like chemical vapor deposition (CVD) or micromechanical cleaving. Existing liquid phase methods suffer from issues such as graphene oxidation during production, layer number dispersion, and small flake size, which significantly compromise the material's overall quality and potential applications.

We present a unique approach using anodic electrochemical exfoliation to synthesize a layer number-monodisperse TG dispersion with exceptional optoelectronic properties comparable to CVD-derived TG. A notable highlight of our research is the high specific capacitance of the film formed from the electrochemically exfoliated TG dispersion, with a specific capacitance of ~ 259 F g^{-1}. This exceptional property positions the TG film as a promising material for capacitive energy storage applications. We have overcome the challenges associated with oxidation and layer number dispersion, achieving large flake sizes. This advancement was possible through an engineered synthesis process guided by in-depth electrochemical characterizations and tight control over experimental parameters during intercalation, exfoliation, and selective cleaving steps. Our research emphasizes the importance of understanding and controlling the electrochemical conditions to yield single-stage III graphite bisulfate, which, upon cleaving in dispersion, favorable solvent results in high-quality TG.

Self-Powered Metal–Semiconductor–Metal 2D WS_2 monolayer Photodetector with Asymmetric Contacts

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Photodetectors are commonly used in many applications, from wireless optical communications to wearable devices. The power consumption in the available devices is high and to minimize power consumption self-powered photodetectors are highly desirable. Herein, we have fabricated a self-powered photodetector based on monolayer WS_2 grown by CVD technique. As grown WS_2 monolayer was characterized by Raman, photoluminescence (PL), and X-ray photoelectron spectrometer, which confirms the high-quality monolayer growth. Two different work-function metals (Ti, 4.3 eV, and Au, 5.1 eV) were used as two electrodes on the monilayer film. The contacts pads were patterned by photolithography and followed by metal deposition using the e-beam evaporation technique. This two metal contacts effectively introduces n and p-doping to monolayer WS_2 creating a lateral PN junction which helps in a higher rectification ratio[1]. The devices showed an excellent on/off ratio of 760 at zero bias for 8.5 mW laser power and a ratio of 3200 at -0.5 V bias for 10 mW laser power. The photodetector has a responsivity of 3.9 A/W and 8.2 A/W corresponding to zero and -0.5 V bias, respectively. The very low dark current in the order of ~ fA helps achieve extremely high detectivity of the order of 10^{17} Jones. The mass production of monolayer WS_2 using CVD or MOCVD will help the way forward for future-generation smart photodetectors.

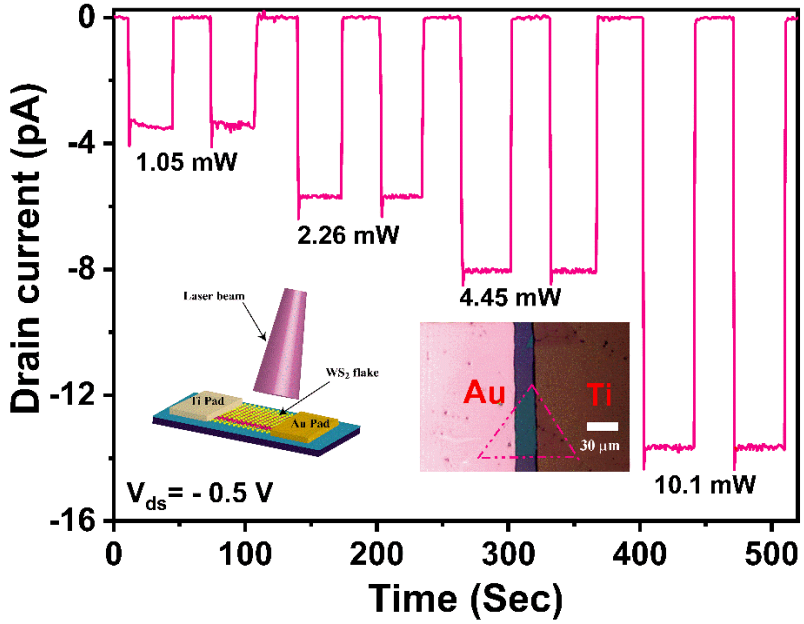

Figure 1. Time response under 405 nm laser excitation with -0.5V bias. Insets are schematic representations and optical images of the final device.

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