

Abstract: 1

A new two dimensional in-plane antiferromagnetic insulator: CoK_2S_2

Anan Bari Sarkar,^{1,*} Barun Ghosh,¹ and Amit Agarwal¹

¹Department of Physics, Indian Institute of Technology, Kanpur-208016, India

Abstract: Two-dimensional (2D) magnetism has been a subject of intensive research in recent times because of their exciting new physics and their potential for applications in the field of electronics and spintronics. Here, we predict a new thermodynamically stable two dimensional magnetic insulator, with an in-plane antiferromagnetic ordering. Bulk CoK_2S_2 shows an antiferromagnetic (AFM) ordering, as observed by neutron diffraction experiment. Our density functional theory (DFT) calculations reveal the presence of flat bands and Van Hove singularities (VHSs) in the density of states near the Fermi energy for the non-magnetic configuration of bulk CoK_2S_2 . Flat bands and VHSs give rise to different many body instabilities, hence the emergence of AFM ordering in bulk. Remarkably, we find that this antiferromagnetic magnetic ordering persists in the monolayer limit as well. To account for the strongly correlated electrons in Co d orbitals, we have used DFT + U scheme for different magnetic orientations in the presence of spin-orbit coupling (SOC). We have found that the in-plane AFM state is the energetically favourable magnetic ground state for non-zero values of U in monolayer CoK_2S_2 . GGA + U + SOC calculations for different spin directions (i.e. along x , y , and z) reveal the presence of an easy spin axis along the chain connecting the cobalt atoms, along with a magneto-crystalline-anisotropy (MAE) energy of the order of 1 meV. This large MAE clearly indicates the robustness of the magnetic ground state even at finite T , in the monolayer structure. Additionally, we also investigate CoK_2S_2 bilayers, and show that the magnetic ground state is AFM with both intra- and inter-layer magnetic coupling being antiferromagnetic.

*Email: sarkar@iitk.ac.in

Abstract: 2

Unusual magneto-resistance of RPdSb (R=Gd, Tb, Ho and Er)

A. Mukhopadhyay and N. Mohapatra

School of Basic Sciences, IIT Bhubaneswar, Odisha, 752050, India

Abstract: We report the results of unusual magnetoresistance (MR) of polycrystalline RPdSb compounds (R=Gd, Tb, Ho and Er). GdPdSb and TbPdSb are found to crystallise in LiGaGe type structure, while HoPdSb and ErPdSb crystallise in cubic MgAgAs type structure. Magnetic characterisation of these compounds shows that GdPdSb, TbPdSb and HoPdSb are antiferromagnetic below 17 K, 2.5 K and 2.2 K respectively. ErPdSb is paramagnetic throughout the temperature of 1.8-300 K. Electrical transport measurement shows that Gd and Tb samples are metallic in nature, whereas the Ho and Er samples are low band gap semiconductors. The most interesting feature is the observation of unusual magnetoresistance (MR) at low temperatures. For Gd and Tb samples, MR is giant, positive, nonsaturating, whereas for Ho and Er samples observed MR is similar to the weak anti-localisation and Alder-Bell-Jackiw anomaly induced feature respectively.

Abstract: 3

Electrically Probing Differently Oriented 1-D Nanostructures via C-AFM

Bikash Das^{1, a)}, Avishek Das¹, Anudeepa Ghosh¹, Ranveer Singh², Sujan Maity¹, Tapobrata Som² and Subhadeep Datta^{1, a)}

¹School of Physical Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata- 700032, India

² Division of Experimental Condensed Matter Physics, Institute of Physics, Bhubaneswar.

^{a)}Corresponding author: intbd@iacs.res.in

Abstract: Electron transport through a nanostructure in source-drain geometry depends on quantum confinement and quality of metal contacts. In addition, transport mechanism varies with the alignment of the nanostructure between the contacts. For potential applications, thorough understanding of the electrical transport of a single nano object having various orientations on the substrate is important but such kind of probing, especially that of a single vertically aligned nanowire having diameter $\sim 20\text{-}100\text{nm} \gg$ length, is technically very difficult even via advanced lithographic techniques. Thanks to atomic force microscopy, current-voltage measurements of a quasi-one dimensional nano-object can be performed using a conductive tip (C-AFM). In the current study, C-AFM has been employed to explore two different transport mechanisms: 1) quantum tunneling in reclined carbon nanotube (CNT) on a conductive surface through the two walls, 2) formation of Schottky barrier in vertical ZnO nanowires due to metal-semiconductor junction. This technique can be employed to probe the defect states and quality of the as grown nanowires.

Abstract: 4

Electronic and optical properties of transition metal doped SnS₂: Bulk, quasi-2D nano-flower and monolayer

Bhagyashri Bhat, Divya Nagaraj, Satishchandra Ogale*, and Mukul Kabir*

Department of Physics, Indian Institute of Science Education and Research, Pune 411008, India

**Centre for Energy Science, Indian Institute of Science Education and Research, Pune 411008, India*

The conversion efficiency of solar energy to electricity in a photovoltaic device is determined by the bandgap of the semiconductor and the concurrent light absorption coefficient. While layered SnS₂ is a wide bandgap indirect semiconductor, transition-metal doping holds enormous promise to engineer its optoelectronic properties. Here, we investigate the electronic, optical and excitonic properties doped SnS₂ crystals with a combination of theoretical and experimental techniques. Theoretical calculations indicate that the metal ions could easily be incorporated within the lattice, and indeed the experimental in-situ doping is done via a one pot facile synthesis process. While most of the doped SnS₂ in all forms remain semiconducting, the band gaps are substantially reduced due to the mid-gap states originating from the TM-3d orbitals. In a few cases, the electronic structure becomes metallic. The optical absorption coefficient is found to be very high above 10⁵ cm⁻¹ due to the proximity of the direct and indirect gaps. The theoretical results are in excellent agreement with the present experimental results. Further, we calculate the exciton binding in these systems to find substantial enhancements in the single-layer due to the inadequate electron screening. Further, we will briefly mention the intriguing magnetic properties of these systems that may be useful for spintronic applications.

Abstract: 5

Plasmon-exciton coupled MoS₂-Au nanostructure for photocatalytic application

Didhiti Bhattacharya¹, Sayan Bayan¹, Rajib K Mira² and Samit K Ray¹

¹Department of Condensed Matter Physics and Material Sciences, ² Department of Chemical, Biological and Macromolecular Sciences

S N Bose National Centre for Basic Sciences

JD Block, Salt Lake, Kolkata 700106, India

email: bhattacharyadidhiti@gmail.com

A metal-semiconductor interface, as in gold(Au)-molybdenum disulfide(MoS₂), is of great interest from the standpoint of fundamental science as it constitutes an outstanding platform to investigate plasmonic-exciton interaction and charge transfer. In this work Au nanoparticle decorated 2H-MoS₂ nanostructure is prepared. The optical properties of Au-MoS₂ nano-hybrids are studied using absorbance, steady state fluorescence, and Raman spectroscopic techniques. Structural analysis of Au-MoS₂ nanohybrids has been done using X-ray diffraction (XRD) and transmission electron microscopy (TEM). The local plasmon resonance of AuNPs and the excitation position of MoS₂ nanosheets are individually observed in this nanostructures and both of them can be tuned as a function of AuNP concentration. Better photocatalytic efficiency of the plasmon-exciton co-driven system is observed than pristine MoS₂ nanosheets in degradation of Brilliant Green dye under visible light irradiation. The photocatalytic degradation rate of Au-MoS₂ is almost 2.5 times greater than pristine MoS₂ nanosheets. Our finding illustrates the potential to control hot carriers for better catalytic reactions by tuning exciton-plasmon coupling between MoS₂ and Au nanoparticles.

Abstract: 6

"Atom-like many body excitonic interaction in large area low symmetric transition metal dichalcogenide"

Dipendranath Mandal

Abstract: 7

MoS₂ quantum dots synthesis and their size modulation by pulsed laser ablation in liquid

Gobinda Pradhan*, Partha P Dey and Ashwini Kumar Sharma

Department of Physics, Indian Institute of Technology Guwahati, Guwahati-781039, India

*Corresponding Author's email: p.gobinda@iitg.ac.in

Abstract:

Recently along with the 2D layered structure, zero-dimensional MoS₂ i.e. MoS₂ QDs has drawn tremendous attention with its additional unique properties compared to the MoS₂ bulk counterpart. As most of the existing QDs like PbSe, PbS, CdAs contains heavy metal which increases the risk of toxic hazards so alternative high efficient nontoxic QDs are in high demand. Hence, MoS₂ QDs which are nontoxic, band gap in the visible region, chemically and thermally stable with a noticeable high efficiency seem to be a good alternative. Among other tedious and time-consuming processes pulsed laser ablation in liquid (PLAL) technique shows a great possibility as an efficient, single step, chemical-free simple physical process to synthesis MoS₂ QDs. In PLAL technique one can tune parameters like laser fluence, laser wavelength, ablation time, liquid medium, etc. Hence a systematic study on the effect of the parameters on the shape and size, concentration of the generated MoS₂ QDs is in scarce. In the present work, MoS₂ QDs are synthesized by PLAL technique with a nanosecond pulsed laser at various laser fluence and ablation time. The effect of laser fluence and ablation time on QDs size and their structures are investigated systematically.

Abstract: 8

Superconductivity in NbN: 2D and 3D

Hemanta Kumar Kundu¹, Kazi Rafsanjani Amin¹, John Jesudasan², Pratap Raychaudhuri²,
Subroto Mukerjee¹, Aweek Bid¹

¹Department of Physics, Indian Institute of Science, Bangalore 560012, India

² Department of Condensed Matter Physics and Materials Science, Tata Institute of
Fundamental Research, Mumbai 400005, India

Despite being at the core of dissipationless transport deep inside the superconducting regime, vortex dynamics in 2D superconductors is not well understood. Here, we present evidence for the existence of a vortex-solid/glass to vortex-fluid transition in a conventional 2D type-II superconductor, NbN, through studies of magnetoresistance and current-voltage characteristics. The dynamical exponents corresponding to this phase transition were extracted independently from the two sets of measurements. The H-T phase diagram for the 2D and 3D superconductors are found to be significantly different near the critical point. The transport properties measured over a broad range of temperature and magnetic fields followed universal scaling relations both in the case of 2D and 3D establishing that the idea of a critical behavior in vortex-solid/glass to vortex-fluid transition is valid for both 2D and 3D superconductors. In the case of 3D superconductor, the exponent values obtained from the two independent measurements show excellent match. On the other hand, for the 2D superconductor, the exponents obtained from the two experiments were significantly different. We attribute this to the fact that the characteristic length scale diverges near the critical point in a 2D superconductor in a distinctly different way from its 3D counterpart.

Abstract: 9

Angle Resolved Photoemission Spectroscopy Study on TaTe₂

Indrani Kar,^{1,*} Luminita Harnagea,² Surjeet Singh,^{2,3} Y. Kushnirenko,⁴ A. V. Fedorov,⁴ N. C. Plumb,⁵ M. Shi⁵ and S. Thirupathaiah¹

¹*Condensed Matter Physics and Material Science Department,
S N Bose National Centre for Basic Sciences, 700106, India*

²*Indian Institute of Science Education and Research,
Dr. Homi Bhabha Road, Pune, Maharashtra-411008, India*

³*Centre for Energy Science, Indian Institute of Science Education and Research,
Dr. Homi Bhabha Road, Pune, Maharashtra-411008, India*

⁴*Leibniz Institute for Solid State Research, IFW Dresden, D-01171 Dresden, Germany*

⁵*Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*

*Corresponding author: karindrani.physics@gmail.com

In the era of thermoelectricity, the thirst of getting new thermoelectric material gave birth to metal-like conductor TaTe₂ along with its similar compounds NbSe₂, NbTe₂, TaSe₂, TaTe₂ [1]. These all belong to transition metal di-chalcogenides (TMDC). Distorted octahedral phase of TaTe₂ (1T'-TaTe₂) shows incommensurate charge density wave (CDW) below ≈ 170 K [2, 3]. Using angle resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) we studied the low-energy electronic structure of bulk TaTe₂ below and above CDW transition temperature (170K). The obtained Fermi surface topology is quite different from its similar compound NbTe₂, TaSe₂ and TaS₂ as reported earlier [4-5]. For the first time using ARPES, we are showing that TaTe₂ is metallic as bands cross the Fermi level. The estimated value of inner potential is 12.89 ± 3 eV from our data. Apart from intensity, the Fermi surface topology has no significant change at high or low temperature whereas previous studies have reported phase transition at around 170 K [3, 6].

References:

[1] L. H. Brixner, Journal of Inorganic and Nuclear Chemistry **24**, 257 (1962).

[2] Y. Liu, D. F. Shao, L. J. Li, W. J. Lu, X. D. Zhu, P. Tong, R. C. Xiao, L. S. Ling, C. Y. Xi, L. Pi, H. F. Tian, H. X. Yang, J. Q. Li, W. H. Song, X. B. Zhu, and Y. P. Sun, Physical Review B **94**, 045131 (2016).

[3] T. Sörgel, J. Nuss, U. Wedig, R. Kremer, and M. Jansen, *Materials Research Bulletin* **41**, 987 (2006).

[4] C. Battaglia, H. Cercellier, F. Clerc, L. Despont, M. G. Garnier, C. Koitzsch, P. Aebi, H. Berger, L. Forró and C. Ambrosch-Draxl, *Physical Review B* **72**, 195114 (2005).

[5] F. Clerc, C. Battaglia, H. Cercellier, C. Monney, H. Berger, L. Despont, M. G. Garnier, and P. Aebi, *Journal of Physics: Condensed Matter* **19**, 355002 (2007).

[6] J. J. Gao, J. G. Si, X. Luo, J. Yan, F. C. Chen, G. T. Lin, L. Hu, R. R. Zhang, P. Tong, W. H. Song, X. B. Zhu, W. J. Lu, and Y. P. Sun, *Physical Review B* **98**, 224104 (2018).

Abstract: 10

Anomalous electronic structure of ReS₂

Joydeep Chatterjee and Priya Mahadevan

Department of Condensed Matter Physics and Materials Sciences

S. N. Bose National Centre for Basic Sciences

While most transition metal dichalcogenides exhibit a strong layer dependence of their bandgap, ReS₂ has been unusual in that it has small variations in its bandgap in going from the monolayer to the bulk limit. In this work we use a combination of ab-initio calculations as well as a mapping of the electronic structure onto a tight-binding model to explain this weak layer dependence. Examining the structure, we find it consists of 4 atom Re clusters connected at their edges and forming one-dimensional chains. The insulating character associated with a formal d³ configuration at the Re site arises because of the strong metal-metal bonding within each cluster. Consequently the valence band maximum and the conduction band minimum are confined primarily in the Re layer, leading to weak interlayer interactions despite the smaller interlayer distance compared to 2H-MoS₂, which shows significant changes with the number of layers.

Abstract: 11

A computational study of sequential deposition: A dynamic monte carlo process in statistical physics

Indranil Ghosh, Budhaditya Banerjee

Jadavpur University, Department of Physics, Post Graduate II,

Email: indranilg49@gmail.com , budhaditya314@gmail.com

Few of the many enthralling applications of dynamic monte carlo process is the study of crystallization of hard spheres due to increase in pressure or the response of Ising model due to an external magnetic field switched on at an initial time, where physical time plays an integral role. In our presentation, we study a phenomenon where particles (discs) are randomly attached to a 2-dimensional surface and stay attached only if they find a required free space. With time, the number of particles that get repelled by other particles, due to not enough free spacing, increases and takes longer time to fill up the surface. We study two algorithms, a naive and then a faster-than-clock algorithm, to simulate this phenomenon of particle saturation, and compare their performances in details. We carry out the simulation with Pygame, a python package. We also calculate the approximate value of the maximum coverage numerically, for these circular particles for different radii after the simulation is carried out for a certain recommended time, with our computer programs. At last we end by investigating how Pygame can be used to carry out simulations of various monte carlo methods in algorithmic statistical physics.

Abstract: 12

Thermoelectric twistrionics at small angle twisted bilayer graphene

Phanibhusan S Mahapatra¹, Bhaskar Ghawri¹, Sujay ray¹, K Watanabe³, T Taniguchi³,
Tanmoy Das¹, Subroto Mukerjee¹, H.R. Krishnamurthy¹, Arindam Ghosh^{1,2}

¹ *Department of Physics, Indian Institute of Science, Bangalore 560 012, India,* ² *Centre for Nano Science & Engineering, Indian Institute of Science, Bangalore 560 012, India,* ³ *National Institute for Materials Science, Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan.*

Introduction of 'twist' or relative rotation between two atomically thin van der Waals (vdW) membranes gives rise to periodic Moiré potential, leading to substantial alteration of the band structure of the planar assembly. These twisted meta-materials, owing to their exceptional tunable nature, have emerged as the ideal platform for studying many novel concepts of condensed matter physics [1,2]. While most of the recent experiments primarily focus on the electronic-wave function reconstruction by probing transport properties in the in-plane direction, we report on thermoelectric measurements across the van der Waals gap in twisted bilayer graphene (t BLG) at small twist angle ($\Theta \sim 0.6^\circ$). The cross-plane Seebeck coefficient shows Lifshitz transitions as the band topology changes from electron-like (hole-like) massless Dirac to hole-like (electron-like) massive bands at the van Hove singularity point. Additionally, we observe temperature dependent splitting and strong non-linearity at both half and quarter filling of the lowest bands even at temperatures $\sim 125\text{K}$, indicating strong electron correlations due to localization of electronic density of states in the system. The twist-controlled cross-plane thermoelectricity in tBLG may provide fundamental insights towards the electron-electron and electron-phonon interactions in Moiré superlattices which can leverage the broad electro structural phase space of layered solids.

Reference:

[1] Cao, Y. *et al.* Correlated insulator behaviour at half filling in magic-angle graphene superlattices. *Nature* **556**, 80 (2018).

[2] Cao, Y. *et al.* Unconventional superconductivity in magic-angle graphene superlattices. *Nature* **556**, 43 (2018).

Engineering spin-valley physics in bilayers of MoSe₂

Poonam Kumari, Joydeep Chatterjee and Priya Mahadevan

S. N. Bose National Center for Basic Sciences, Kolkata

Spin-orbit interactions lead to a large spin-splitting of the valence band maximum at K in MoSe₂ monolayer. However, on stacking a second layer of MoSe₂ in the same manner (2H) as found in the bulk, one finds that there is no net spin splitting, which has been attributed to inversion symmetry. An obvious route to making the bilayers useful for exploring the coupled spin and valley physics is through breaking inversion symmetry. We examined this by rotating the top layer by an angle θ with respect to the lower layer. We find that for some angles of rotation, the spin splitting vanishes, even though there is no inversion symmetry in these structures. In this work we demonstrate and explain a mechanism for vanishing of the spin-splitting in these systems where the hexagonal symmetry of the lattice brings about an unexpected dependence of the electronic structure on the angle of rotation. The unusual electronic structure for the twisted bilayer graphene has led to the observation of superconductivity there. Hence any simplification of the electronic structure of the twisted bilayers which involve huge unit cells as in the present work allows us to explore regimes beyond those possible in first principle calculation.

Abstract: 14

Exploring Spin Valley Physics in Bilayers of MoS₂

Prasun Boyal¹ and Priya Mahadevan¹

S N Bose National Centre for Basic Sciences

Email: prasun.boyal@gmail.com

Abstract:

Bilayers of MoS₂ in the stacking that is found in the bulk have their valence band maximum at Γ point as well as have no net spin splitting at the K point. The former is attributed to the interaction between the out of plane orbitals of the two layers. One way to bring the valence band maximum back to K point in bilayers is by applying bi-axial compressive strain to increase the interaction between in plane orbitals. We determined the amount of strain required to shift the valence band maximum from Γ point back to K point. This is found to be at 3.5%. Alternate strategies to reduce the strain will be presented. As the presence of inversion symmetry results in the vanishing spin splitting, we will use twisted bilayers to result in a net spin splitting.

Abstract: 15

Real-time observation of spin-resolved exciton-plasmon polaritons in metal-TMDs hybrids

Rup K Chowdhury¹, Shivakiran BN Bhaktha¹ and Samit K Ray*^{1, 2}

¹Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur - 721302, India

²S. N. Bose National Centre for Basic Sciences, Kolkata - 700106, India

Strong light-matter interactions between resonantly coupled metal plasmons and spin decoupled bright excitons from two dimensional (2D) transition metal dichalcogenides (TMDs) can produce unique spin-resolved exciton-plasmon polariton (plexciton). A few efforts have been made to perceive the spin induced exciton-polaritons in nanocavities at cryogenic conditions, however, successful realization of spin-resolved plexciton in time-domain is still lacking. Here, we report both the spin-resolved plexcitons discretely at room temperature and investigate their ultrafast temporal dynamics in size-tunable Au-WS₂ hybrid nanostructures using femtosecond pump-probe spectroscopy technique. Furthermore, a zero detuning between the excitons and plasmons is achieved at ~ 7.0 ps along with a transient Rabi-splitting energy exceeding ~ 250 meV for both the spin-plexcitons, validating the strong-coupling conditions of polariton formation. Realization of these novel spin-plexcitons in scalable metal-TMDs platform, therefore, open up fascinating pathways for both fundamental understanding and their state-of-the-art applications in quantum photonics operating at room temperature.

Abstract: 16

ENHANCEMENT OF INTERFACIAL THERMAL CONDUCTANCE IN HEXAGONAL BORON NITRIDE (h-BN)-GRAPHENE HETEROSTRUCTURES

Saheb Karak¹, Suvodeep Paul¹, Devesh Negi¹, Bommareddy Poojitha¹, Saurabh
Srivastava², Anindya Das² and Surajit Saha¹

¹Department of Physics, Indian Institute of Science Education and Research, Bhopal, India

²Department of Physics, Indian Institute of Science, Bengaluru, India

Email Id: saheb@iiserb.ac.in

Atomically thin monolayers of graphene show unique properties which have led to a great deal of research on their use in nanoscale devices. Graphene on h-BN substrate has been reported to show enhanced (opto) electronic and thermal properties as compared to SiO₂/Si supported graphene. However, heat management of such nanoscale devices is essential in order to improve their performance. Motivated by this we have performed temperature and power dependent Raman Spectroscopic measurements on different types of (hetero) structures: (a) h-BN, (b) Graphene, (c)h-BN on Graphene, and (d)graphene encapsulated by two h-BN layers, all supported on SiO₂/Si substrate. We have estimated the value of thermal conductivity (κ) and interfacial thermal conductance per unit area (g) of these four (hetero) structures. We measure the values of κ and g for h-BN supported on SiO₂/Si. Further, we have observed an improvement in both κ and g in the hetero-structures, ensures a better heat dissipation in devices. The κ and g of h-BN encapsulated graphene sample were observed to be 850 Wm⁻¹K⁻¹ and 14.7±0.8 MWm⁻²K⁻¹, respectively, as opposed to 600 Wm⁻¹K⁻¹ and 1.15 MWm⁻²K⁻¹, respectively, for graphene on SiO₂/Si substrate. Therefore, we propose that for graphene-based nanoscale devices, encapsulation with h-BN is a better alternative to address heat management issues.

Fig: Intensity profile of 2D and h-BN mode for (a-d) heterostructures.

References:

1. A. C. Ferrari *et al.* Nature Nanotech. **8**, 235 (2013)
2. A. A. Balandin *et al.* Nano. Lett. **8**, 902 (2008)

Abstract: 17

Fabrication of two-dimensional van der Waal heterostructure and bilayer graphene transistor

**Shubhadip Moulick¹, Shubhrasish Mukherjee¹, Sreyan Raha², Achintya Singha²
S. K. Ray¹ and Atindra Nath Pal¹**

¹*Condensed Matter Physics and Material Sciences, SNBNCBS*

²*Department of Physics, Bose Institute*

moulick.shubhadip94@gmail.com

Two dimensional materials like graphene or various TMDCs (MoS₂, WS₂ etc.) have shown lot of promises due to their excellent electronic, optical and mechanical properties. In the last few years there are several attempts to combine these materials to create new functional device. These hybrid structure combine different properties of materials resulting into improved performance of the combined device, which cannot be accomplished from a single material. 2D van der Waals materials has very strong covalent bond among the atoms present in them; however the weak interaction between the two 2D layer ensure stacking of two different materials ensuring unaltered material properties. Several interesting phenomena like Hofstadter Butterfly [1], Valley Hall effect [2], Coulomb drag [3] were observed in graphene-Boron Nitride heterostructure. Similarly, graphene on MoS₂ binary heterostructure shows dual optoelectronic property including highly sensitive photo detection and gate tunable photoconductivity [4]. Here we have developed the way to stack the atomically thin Van Der Waals materials to make desired hybrid structure using a simple microscope based set up. The set up consists of a customized heater stage and it has been optimized to pick up a 2D layer (graphene, hBN, MoS₂ etc.) from PDMS or SiO₂ substrate and can be transferred to a desired surface.

The same set up has been used to fabricate a top gated bilayer graphene transistor. A bilayer graphene was identified and transferred to a predefined contacts. Then ionic gel is used as a top gate dielectric. Simultaneous electrical conductance measurement and in situ Raman spectroscopy were performed in this device. We observed a large tunability with the gate voltage and a consistent shift in the G peak of the Raman spectrum, which signifies a tunable electron-phonon interaction by the application of gate voltage.

References

1. B. Hunt¹, J. D. Sanchez-Yamagishi¹, A. F. Young, M. Yankowitz, B. J. LeRoy, K. Watanabe³, T. Taniguchi³, P. Moon, “Massive Dirac Fermions and Hofstadter Butterfly in a van der Waals Heterostructure.” *Science* 21 Jun 2013:Vol. 340, Issue 6139, pp. 1427-1430
2. Katsuyoshi Komatsu¹, Yoshifumi Morita², Eiichiro Watanabe³, Daiju Tsuya³, Kenji Watanabe⁴, Takashi Taniguchi⁴,” Observation of the quantum valley Hall state in ballistic graphene superlattices”, *Science Advances* 18 May 2018:Vol. 4, no. 5, eaag0194
3. J. I. A. Li, T. Taniguchi, K. Watanabe, J. Hone, A. Levchenko, and C. R. Dean,” Negative Coulomb Drag in Double Bilayer Graphene”, *Phys. Rev. Lett.* 117, 046802
4. Kallol Roy, Medini Padmanabhan, Srijit Goswami, T. Phanindra Sai, Gopalakrishnan Ramalingam Srinivasan Raghavan & Arindam Ghosh “Graphene- MoS₂ hybrid structure for multifunctional photoresponsive memory devices” *Nature Nanotechnology* 8, 826-830 (2013).

Abstract: 18

Size Tunable Optical Properties of Black Phosphorus Nanoparticles Synthesized via Sono-chemical Exfoliation

**Subhajit Jana^{1,*}, Subhrajit Mukherjee¹, Arup Ghorai², Shivakiran B. N. Bhaktha¹
and Samit K. Ray^{1,3}**

¹*Department of Physics, Indian Institute of Technology, Kharagpur, WB, Pin-721302, India*

²*School of Nanoscience and Technology, Indian Institute of Technology, Kharagpur, WB,
Pin-721302, India*

³*Currently at S. N. Bose National Centre for Basic Sciences, Kolkata, WB, Pin-700106, India*

**Presenting author: subhajitphy@iitkgp.ac.in*

Black phosphorus (BP), a relatively new member to 2D material community has drawn tremendous interest of researchers due to its direct and size tunable band gap [1]. Among different synthesis methods, chemical synthesis routes are very promising to synthesize various 2D materials as they give large number of flakes together with variable layer number [2]. Here we report synthesis of electronic grade, highly luminescent few layer black phosphorus nanoparticles (BPNPs) in a simple sono-chemical exfoliation method. Various characterization techniques like TEM, AFM and Raman spectroscopy have confirmed the exfoliation of bulk black phosphorus to few layer BPNPs. Size tunable absorption and emission properties of as synthesized sample have been studied thoroughly. Instability of bare BPNP in ambient atmosphere was seen as they rapidly get oxidized whenever air exposure happened as further confirmed by XPS spectra. As the temperature decreases, near band-edge optical transitions become more prominent than others originated from various functional groups. Most interestingly, BPNPs with relatively larger size show a transition from mixed thermal quenching behaviour to positive thermal quenching and in contrary relatively smaller size NPs show negative thermal quenching.

References:

[1] F. Xia, H. Wang, D. Xiao, M. Dubey, and A. Ramasubramaniam, “Two-dimensional material nanophotonics,” *Nat. Photonics*, vol. 8, no. 12, pp. 899–907, 2014.

[2] A. H. Woomer, T. W. Farnsworth, J. Hu, R. A. Wells, C. L. Donley, and S. C. Warren, “Phosphorene: Synthesis, Scale-Up, and Quantitative Optical Spectroscopy,” *ACS Nano*, vol. 9, no. 9, pp. 8869–8884, 2015.

Influence of Single Walled Carbon Nanotubes on the Ideality Factor of Rose Bengal Dye Based Organic Device

Sudipta Sen*, Nabin Baran Manik

Condensed Matter Physics Research Centre, Department of Physics

Jadavpur University, Kolkata- 700032, India

*E-mail: sagnike000@gmail.com

Abstract

Organic devices are getting much more attention nowadays due to their flexibility, cost effectiveness and easy fabrication process over a large area [1]. Despite these advantages, there are also certain limitations of organic devices. One of the major limitations is the high threshold voltage of the device which can be attributed to its high ideality factor. Attempts regarding the reduction of the ideality factor will improve the device performance and also the device can be turned on at much lower voltage. In this work, we have studied the ideality factor of ITO coated glass/ Rose Bengal (RB) dye /Aluminium based organic device and subsequently we have also observed the effect of single walled carbon nanotubes (SWCNT) on ideality factor. We have used ITO coated glass as front electrode and aluminium as back electrode to form the organic device. This organic device has been prepared with and without SWCNT by using spin coating technique [2]. We have measured the steady state current-voltage (I-V) characteristics of the device to estimate the threshold voltage and ideality factor of the device. Threshold voltage is reduced from 3.11 V to 1.89 V and ideality factor is reduced from 29.01 to 11.35 in the presence of SWCNT. Incorporation of SWCNT provides an extra charge percolation path in the device due to which both threshold voltage and ideality factor are reduced. It indicates that the device can be turned on at much lower voltage and the device performance will also be improved in the presence of SWCNT. This work shows that by suitable doping or addition of SWCNT within the RB dye it is possible to control the threshold voltage and also the ideality factor of the device.

Keywords: Ideality Factor; Rose Bengal Dye; SWCNT; Threshold voltage

REFERENCES:

[1] S. Chakraborty, N. B. Manik, *Physica B*. 481 (209) (2016)

[2] K.Chakraborty, S.Chakraborty, N. B. Manik, *J.Semicond.* 39(9) (2018)

Evolution of inter-layer coupling in artificially stacked MoS₂ layers

Suman Sarkar¹, H L Pradeepa¹, Goutham Nayak², Indrajit Maity¹, Laetitia Marty², Julien Renard², Johann Coraux², Nedjma Bendiab², Vincent Bouchiat², Jaydeep K Basu¹, Manish Jain¹ and Aweek Bid¹.

¹Department of Physics, Indian Institute of Science, Bangalore 560012, India.

²Univ.Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France.

The fabrication of atomically-clean interface of van der Waals material is essential to probe their proposed exotic properties and for their applications in next generation optoelectronic devices. We show that the hybridization of bands of adjacent layers is possible only for van der Waals heterostructures with ultraclean interfaces. This we achieve through detailed experimental studies and analysis of the effect of interface separation and the amount of adsorbates at the interface on photoluminescence and Raman spectra. For ultra-clean interfaces, the vibrational modes and optical responses differ significantly from those of the constituent layers. For such systems, we observe a shift in Raman spectra from that of individual constituent layers, the appearance of inter-layer low frequency breathing modes, quenching of the photoluminescence signal and appearance of an indirect peak in photoluminescence spectra. Our study establishes that it is possible to engineer van der Waals heterostructures with desired optical properties by controlling the inter-layer spacing, and consequently the interlayer coupling between the constituent layers.

Abstract: 21

Layer dependence of the electronic structure of transition metal dichalcogenides

Sumanti Patra¹ D.D. Sarma² and Priya Mahadevan¹

¹Department of Condensed Matter Physics and Material Science, S. N. Bose National Centre for Basic Sciences, Kolkata-700106

²Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore.

The size dependence of the electronic properties of semiconductor nanocrystals have been investigated for many years [1]. The sizes up to which one has a deviation in the electronic structure from the bulk limit depend on the Bohr radius of the semiconductors. The recent interest in the two dimensional transition metal dichalcogenides has led to an analogous question being asked for this class of materials which have weak van der Waals interactions between the layers. In this work we will present a microscopic model which captures the behaviour and discusses the origin.

References:

[1]. Viswanatha, Ranjani, et al. *Physical Review B* 72.4 (2005): 045333.

Abstract: 22

ARPES Study on Magnetically Doped Topological Insulator Bi_2Se_3

Susmita Changdar¹, Rabia Sultana², Soma Banik^{3, 4}, V. P. S. Awana², and Setti Thirupathaiah¹

¹Condensed Matter Physics and Material Sciences department, S N Bose National Centre for Basic Sciences, JD Block, Sector – III, Salt Lake, Kolkata-700106, India.

²CSIR-National Physical Laboratory, Dr KS Krishnan Marg, Pusa, New Delhi, Delhi 110012

³Synchrotron Utilization Section, Raja Ramanna Centre for Advanced Technology, Indore, 452013, India.

⁴Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai, 400094, India.

* Corresponding author: changdar.susmita@gmail.com

Theoretically, it has been predicted that, presence of magnetic ordering in topological insulators (TIs) can cause band gap opening at the Dirac point by breaking the time reversal symmetry (TRS). For experimental observation of the effect on electronic band structure in presence of magnetic impurities, we have done high-resolution angle-resolved photoemission spectroscopy (ARPES) study on 3D TI Bi_2Se_3 and its magnetically doped compounds, $\text{Co}_{0.1}\text{Bi}_2\text{Se}_3$, $\text{Mn}_{0.1}\text{Bi}_2\text{Se}_3$ and $\text{Eu}_{0.1}\text{Bi}_{1.9}\text{Se}_3$. Though no band gap opened up at the Dirac point for small amount of doping, shift of the Dirac point towards higher binding energy was observed. Our measurements show conducting surface and insulating bulk states in all the compounds and also indicate that doped magnetic elements donates additional electrons to the Bi_2Se_3 , which eventually causes shift of the Dirac point.

Phonon anomalies in 1T'-MoTe₂

Suvodeep Paul, Saheb Karak, Manasi Mandal, R.P.Singh, and Surajit Saha.
Department of Physics, Indian Institute of Science Education and Research, Bhopal

Transition metal dichalcogenides (TMDs) exist in a variety of polymorphs among which the semiconducting 2H phase has been explored well. Recent studies on the other phases, however, revealed many exciting findings. The 1T' phase of TMDs has been predicted to be topological spin hall insulators [1]. Further, 1T'-MoTe₂ has been reported to undergo a phase transition at ~250 K to a type-II Weyl semi-metallic Td phase [2]. The requirement of Weyl semimetals is the breaking of the crystal inversion symmetry which can be studied very accurately by techniques like Raman spectroscopy [3]. We have conducted Raman spectroscopic studies on single crystals of 1T'-MoTe₂ in order to study the phase transition. Besides, we have observed anomalous traits in the temperature behaviour of certain phonons which might be attributed to electron-phonon coupling. Further, studies on exfoliated flakes reveal the absence of any crystal inversion symmetry breaking in the thin flakes, confirming the stabilization of the 1T' phase for all exfoliated flakes below a critical thickness, contrary to previous reports [4]. Finally, we have observed a reduction in electron-phonon coupling with the decrease in flake thickness. These observations can be explained very well by the hole doping in the thin flakes induced by exposure to atmospheric oxygen.

References:

1. X. Qian *et al.*, *Science* **346**, 1344 (2014).
2. R. Clarke *et al.*, *Phil. Mag.* **B38**, 121 (1978).
3. K. Zhang *et al.*, *Nat. Commun.* **7**, 13552(2016).
4. R. He *et al.*, *Phys. Rev.* **B97**, 041410 (2018).

Abstract: 24

High Responsive Silicon based Heterojunction Photodetectors using Graphene Quantum Dots as UV photon harvester

Tamal Dey^{1*}, Arup Ghorai¹, Soumen Das² and Samit Kumar Ray^{3,4}

¹*School of Nanoscience and Technology, Indian Institute of Technology, Kharagpur, India,*

²*School of Medical Science and Technology, Indian Institute of Technology, Kharagpur, India*

³*Department of Physics, Indian Institute of Technology, Kharagpur, India,*

⁴*S.N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata.*

*Presenting author: tamald40@gmail.com

Ultraviolet photodetectors have tremendous importance in safety measures against increasing UV radiation on earth surface, warning systems used in missiles or aviation industry, various biological and chemical sensors etc. Traditional UV detectors made of large band gap semiconductors require high temperature costly processing. Silicon detectors suffer from thermalization of charge carriers at UV regime. Hence, Graphene Quantum Dots (GQD), a material which has excellent UV absorption and can be processed by cost effective solution processed technique¹, is increasingly being utilized in various optoelectronics application². GQDs absorb UV light and emit longer wavelength photons with high PL quantum yield. Hence GQD/silicon heterojunction exhibits high responsivity in the UV, contrary to the traditional silicon commercial photodetector. It has been observed that size of GQDs play important role in the charge transfer mechanisms for optimal device performance. Photo generated carrier lifetimes were measured by Photoluminescence decay experiment. Two factors play role in the lifetime of the photo generated carriers, (a) excitonic oscillator strength, (b) non-radiative fast recombination centres, both are dependent on size of GQDs and are competing in nature. Taking them both into account, optimized sized GQDs were used for device fabrication. The devices show high responsivity in the UV, compared to commercial silicon photodetectors. The devices exhibit photo-to-dark current ratio of ~2000 and fast switching under ON/OFF conditions.

References:

[1] Pan, Dengyu, et al. "Hydrothermal route for cutting graphene sheets into blue-luminescent graphene quantum dots." *Advanced materials* 22.6 (2010): 734-738.

[2] Zhang, Qing, et al. "Solution-processed graphene quantum dot deep-UV photodetectors." *ACS nano* 9.2 (2015): 1561-1570.

