Abstract: 1

Optical Properties of Plasmon–Coupled 2D Materials

Achintya Singha[1*], Tara Shankar Bhattacharya[1], Sreemanta Mitra[1], Shib Shankar Singha[1], Prasanna Kr. Mondal [2]

[1]Department of Physics, Bose Institute, 93/1, A.P.C Road, Kolkata, 700009, India.

[2]Department of Physics, Surendranath College, 24/2 M. G. Road, Kolkata 700009, India

*Email: achintya@jcbose.ac.in

Recently, considerable attention has been paid to tune the emission using hybrid systems composed of 2D materials and metal nanoparticles (NPs) since NPs have the ability to enhance and localize the incident electromagnetic field. Furthermore, these hybrid systems show great interest from the standpoint of fundamental science as it constitutes an excellent platform to investigate light-matter interaction [1-3].

Here we realized WS_2-Au NP hybrids by chemically growing Au NPs at the edges of the mechanically exfoliated bilayer WS_2. Huge enhancement of the PL intensity in the WS_2 - Au composite concerning the pristine WS_2 has been observed, and it increases as the number and size of the Au NPs on WS_2 is increased. Geometry dependent modification of plasmon resonance energy of Au NP alters the coupling strength between the emission pathways of WS_2 and plasmon which is manifested by a change of relative intensity between trion and exciton emissions [4]. We probe the mechanism of the PL intensity modulation through polarization dependent measurements and simulation. We have demonstrated that in WS_2 the internal quantum efficiency increase and activation energy decreases due to coupling with Au NPs. Compared to pristine WS_2, a faster change of optical bandgap with temperature in WS_2-Au may be due to enhancing electron-phonon interaction and lattice expansion in the later.

References:

1. K. Okamoto et al.,Nat. Mater. 3,601 (2004).

2. B. Lee et al., Nano Letters 15, 3646 (2015).

3. Z.Wang et al., Nat. Comm. 7, 11283(2016).

4. T. Bhattacharya et al., manuscript submitted

Abstract: 2

Non-linear optical response in graphene

Amit Agarwal

amitag@iitk.ac.in

Abstract: 3

Spin effects at the boundary of graphene

Arindam Ghosh, IISc Bangalore

arindam@iisc.ac.in

The edge topology and localized defects in a physically finite graphene layers are predicted to host novel charge and spin states. For example, the zigzag (ZZ) edge of both single and bilayer graphene is a perfect one dimensional (1D) conductor due to a set of zero energy gapless states that are topologically protected against backscattering. Competing effects of edge topology and electron-electron interaction in these channels have been probed with scanning probe microscopy, which reveals geometry-dependent magnetic order. Magnetic order is also predicted in graphene with topological line defects, hydrogen chemisorption and point defects with larger carbon rings along grain boundaries. In this talk, I shall demonstrate novel experimental approaches toward probing magnetic state at the graphene boundary with electrical transport. Two classes of boundaries will be addressed: (1) Mechanically exfoliated edges of single and bilayer graphene [1,2], and (2) individual grain boundaries between two crystallites of single layer graphene created by chemical vapour deposition [3]. We find the magnetic order at the edge of gapped single and bilayer graphene leads to hysteretic magneto-transport. At the graphene grain boundaries, on the other hand, we find unambiguous signature of spontaneous breaking of time reversal symmetry at low temperatures (below 1 K), which is a characteristic feature of frozen magnetic order. Dependence on temperature and doping suggests that such an order may develop from the interaction between defect-bound magnetic moment at the grain boundaries and Dirac electrons/holes in graphene. Our experiments suggest a new resource for magnetism in graphene-based low-dimensional structures.

References:

[1] A. Kinikar, T. P. Sai, S. Bhattacharyya, A. Agarwala, T. Biswas, S. Sarker, H. R. Krishnamurthy, M. Jain, V. Shenoy, A. Ghosh, Nature Nanotechnology (2017) doi:10.1038/nnano.2017.24.
[2] M. A. Aamir, P. Karnatak, A. Jayaraman, T. P. Sai, T. V. Ramakrishnan, R. Sensarma, and A. Ghosh Phys. Rev. Lett. 121, 136806 (2018).
[3] Kimberly Hsieh et al. (Under preparation)

Abstract: 4

Non-local transport in InAs/GaSb composite quantum well

Atindra Nath Pal, SNBNCBS, Kolkata

atin@bose.res.in

There is a growing interest in the InAs/GaSb composite quantum well sandwiched between two Al Sb barriers because of its unique band alignment. In this hybrid system an electron layer in InAs can coexist with a hole layer in the GaSb and a hybridization gap is expected to occur due to quantum tunnelling between the layers. Depending on the QWs' thicknesses and on the perpendicular electric field, a rich phase diagram is predicted. It should be possible to electrically tune the sample from standard conducting phases to insulating, semimetallic, or topological,insulator.phases.

In this talk, I will present transport measurements in a Hall bar device where it was possible to observe both electron and hole transport by tuning a top gate voltage. At high magnetic field we observe well defined quantum Hall plateaus for both electron and holes, indicating the good quality of the sample. Surprisingly, at the charge neutrality point we observe that the longitudinal resistivity increases to much higher than the resistance quantum, together with a strong non-local resistance of similar magnitude. We explain our observation with a model which includes the existence of counter propagating dissipative edge channels coupled with residual bulk scattering. Finally I will show our recent measurements on the mesoscopic devices, where we observe signature of ballistic transport, boundary scattering and discuss how the fabrication process influences the electronic transport in these devices.

Abstract: 5

Polariton devices in van der Waals materials

Biswanath Chakraborthy

biswanath.chakraborty@gmail.com

Abstract: 6

Chemically exfoliated few layer MoS_2: What do we understand of its properties

D. D. Sarma
Solid State and Structural Chemistry Unit
Indian Institute of Science, Bengaluru 560012

A metastable phase, existing only as small patches in chemically exfoliated few-layer, thermodynamically stable 2H phase of MoS_2 is believed to influence critically properties of MoS_2 based devices. Its electronic structure is little understood in absence of any direct experimental data and conflicting claims from theoretical investigations. Different publications report conflicting transport properties with suggestions of both being metallic and semiconducting. I shall present data[1,2] to conclusively resolve this issue based on probing the electronic structure of chemically exfoliated few layer systems using spatially resolved photoemission spectroscopy and show that the dominant belief of a metallic 1T phase is qualitatively incorrect and the phase formed is essentially the small-gap semiconducting 1T'. Our results also explain under what circumstances the system may show metallic conduction.

This work is carried out in collaboration with Banabir Pal, Anjali Singh, Sharada. G, Pratibha Mahale, Abhinav Kumar, S. Thirupathaiah, H. Sezen, M. Amati, Luca Gregoratti, Umesh V. Waghmare, Debasmita Pariari, Mit Naik, Rahul Varma, Maya Nair, Arindam Ghosh, and Manish Jain.

References:

1. Banabir Pal *et al*., Phys. Rev. B 96, 195426 (2017).

2. Debasmita Pariari *et al*., Unpublished results.

Abstract: 7

Excitons in flatland

K.V.Adarsh

adarsh@iiserb.ac.in

Abstract: 8

Efficient non-radiative energy transfer across layered heterojunctions

Kaushik Majumder

kausikm@iisc.ac.in

Speaker: Kausik Majumdar, Department of Electrical Communication Engineering, Indian Institute of Science, Bangalore 560 012

Abstract: Monolayers of transition-metal dichalcogenides exhibit a variety excitonic states. These near-two-dimensional excitons are markedly different from typical exciton states observed in three-dimensional bulk semiconductors and their quantum wells, in terms of binding energy and spontaneous emission rate. This makes these monolayers an ideal platform to study exciton physics. In this talk, I shall discuss our recent works on how energy can be efficiently transferred from one layered material into another through such excitonic states due to the spatial proximity and favoured dipole orientation between two layers in a van der Waals heterojunction. Direct implications of such efficient dipole-induced energy transfer will be discussed in terms of strong enhancement of photoluminescence (both single-photon and two-photon) and Raman signals, as well as generation of strong photocurrent from such vertical heterostructures.

Abstract: 9

2D superconductivity and quantum metal phase in 1T-MoS2

Madhu Thalakulam, IISER Thiruvananthapuram

madhu@iisertvm.ac.in

The Berezinskii-Kosterlitz-Thouless phase transition and Bose metal phase, driven by vortices and their dynamics are the hallmark features of a clean two-dimensional superconductor. Materials with a minimal structural disorder and high conductivity are essential for the observation of these features. 1T-MoS2, a relatively unexplored metallic van der Waals material, is a promising candidate in this regard. We observe two-dimensional superconductivity on a few-layer 1T-MoS2 device. The electrical characterisation reveals a transition temperature T_c ~920 mK. Berezinskii-Kosterlitz-Thouless transition and anisotropy in the magneto-transport confirm the dimensionality of the superconductivity. In addition, we observe an enhancement in the parallel upper-critical-field and emergence of the Bose metal state in our sample. The observation of 2D superconductivity in 1T-MoS2 and the capability to scalably engineer this phase on the semiconducting 2H-MoS2 phase opens up a new route for the realization and study of monolithic hybrid quantum circuits.

Abstract: 10

Correct description of MPX$_3$ trichalcogenides in DFT : A case study

Prasenjit Sen (HRI)

prasen@hri.res.in

Abstract: With much current interest in layered materials, ternary transition metal tri-chalcogenides (general formula MAX$_3$, M=TM, A=Si, Ge or P, X=S, Se or Te) are receiving renewed attention. A subset of these compounds are found in layered structures. Most of these are magnetic semiconductors with sizable band gaps (1.5-3 eV) making them attractive in various applications. Mono- to a few-layers of these compounds have been successfully exfoliated and studied.
On the theoretical front, attempts are being made to identify easily `exfoliable' layered materials using high throughput computational approaches. A few theoretical works have reported on these tri-chalcogenides. However, two of these failed to get the correct ground state for the well characterized (A=P) compound FePSe$_3$. Others did not provide sufficient details for a comparison with experimental literature.
Given this scenario we undertake a DFT study of four well studied compounds in this family- MnPS$_3$, MnPSe$_3$, FePS$_3$ and FePSe$_3$- and try to understand what it takes to correctly describe the electronic and magnetic structure of these materials. I will present our results on how we arrive at correct description of all the compounds, most importantly of FePSe$_3$. I also discuss the insights we obtain into the relation between structural, and electronic and magnetic properties of these compounds. Importance of these results in the context of high throughput computational approaches will be mentioned.

Abstract: 11

Unexpected symmetries in twisted bilayer MoSe2

Priya Mahadevan[1]

[1]*S. N. Bose National Centre for Basic Sciences, Kolkata, India*

Spin-orbit interactions lead to a large spin-splitting of the valence band maximum at K in MoSe2 monolayers. 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. This has been attributed to the presence of inversion symmetry. As exploiting the spin splitting at the K valleys allows us to increase the functionality, 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 of the bilayer by an angle θ with respect to the lower layer. The choice of angles was restricted to those for which one had reasonable sized supercells and were otherwise arbitrary. Surprisingly, we found several instances where the spin splitting vanished, though there was no breaking of inversion symmetry. An unusual mechanism behind this is identified. Additionally we found that while the spin splitting existed for θ, it vanished for 60-θ. This unusual behavior, we find, is a consequence of the symmetry of the hexagonal Brillouin zone.

This is work done in collaboration with Poonam Kumari and Joydeep Chatterjee.

Abstract: 12

Light matter interactions in plasmonic hybrid WS2 layers

S. K. Ray

samit@bose.res.in

Abstract: 13

Hybrid mechanical resonators with graphene

Saikat Ghosh

saikat01@gmail.com

Abstract: 14

Exploring the interplay between surface and bulk conductivity in Bi_2Se_3 and the role of disorder, using a sensitive non contact technique

Satyajit Banerjee
Dept. of Physics, IIT Kanpur
email: satyajit@iitk.ac.in

Presence of non-magnetic disorder in Topological insulator's (TI's) often dopes the material with extra electrical charges, thereby creating a normal electron fluid coexisting along with the exotic Dirac electron fluid. As both these fluids contribute to parallel electrical conduction channels, hence conventional electrical transport measurements are not convenient experimental tools for identifying the Dirac electron fluids and exploring their useful properties. We have developed [[1]]a novel technique wherein a popular TI material with disorder, namely Bi_2Se_3 with Se vacancies in the atomic crystal lattice, is used to inductively couple the response between two coils. Through this setup we are not only able to specifically identify the contribution from currents electromagnetically induced in the TI's Dirac electron fluid, but also unravel a complex temperature dependent interplay between the two fluids [1,2].

References:

[1] Amit Jash, Kamalika Nath, T.R. Devidas, A. Bharathi, and S.S. Banerjee, Phys. Rev. Applied 12, 014056 (2019).
2. Amit Jash, Sayantan Ghosh, A. Bharathi, and S.S. Banerjee, (ms under preparation (2019).

Abstract: 15

Excitons in Flatland

Sajal Dhara

Department of Physics, IIT Kharagpur,

Kharagpur-721302

Abstract:

Excitons in two dimensional materials gained a lot of attention in semiconductor optoelectronics in recent time. Underlying lattice structure imposes additional quantum degree of freedom to electronic states known as valleys that can be manipulated optically. Strong spin-orbit splitting of energy bands in some transition metal dichalcogenides gives rise to the effect of valley coherence. Light-matter coupling not only produces the exciton-polariton modes but it can also preserve the valley coherence effect. In this talk, I would focus on the valley physics and light-matter interaction using monolayer thick transition metal dichalcogenides (TMDC) embedded in an optical microcavity. Some of our most recent experimental results in 2D materials would also be presented.

Abstract: 16

Photodetection using few-layer TMDs and their heterostructures

Saurabh Lodha
Professor, Department of Electrical Engineering
Indian Institute of Technology Bombay

Abstract: Recent years have witnessed explosive growth in research on two-dimensional (2D) van der Waals (vdW) materials. A large array of materials with varying properties can benefit applications ranging from electronics and optoelectronics to sensing and spintronics. This talk will describe ongoing experimental efforts in our group on engineering the photodetection performance of optoelectronic devices based on layered 2D vdW semiconductors and their heterostructures.

Ultra-thin 2D transition metal dichalcogenide semiconductors, such as MoS_2, not only promise excellent short-channel control for sub-10 nm logic transistors but also exhibit a large photoresponse, high optical absorption, tunability of the band gap and high flexibility coupled with the ability to form defect-free heterointerfaces, making them highly attractive for a wide range of optoelectronic applications. Experimental results highlighting the trade-off between responsivity and speed in gated vdW ReS_2 photodetectors through modulation of extrinsic and intrinsic trap concentrations will be presented. Recent results on the photoresponse, including the photovoltaic effect, of WSe_2/ReS_2 p-n heterojunction diodes and on engineering photo-amplification in electrostatically doped WSe_2 n-p-n and interdigitated phototransistors will also be discussed.

Bio: Prof. Saurabh Lodha graduated from IIT Bombay in 1999 with a B. Tech (EE) followed by a Masters (ECE) and PhD (ECE) from Purdue University in 2001 and 2004 respectively. His graduate research focused on III-V metal/semiconductor interfaces and molecular electronics. From 2005-2010 he worked at Intel Corporation in Portland, USA, where he was part of the team responsible for the research and development of 45, 32 and 22 Si CMOS process technologies. He joined IIT Bombay in July 2010 where he is currently Professor of Electrical Engineering, PI of the nanofabrication facility and co-PI of IIT Bombay's Research Park. He has been awarded the Swarnajayanti fellowship by DST and young investigator and best research paper awards by IIT Bombay. His research interests span devices and materials in the areas of advanced CMOS technologies, 2D (opto)electronics, Si photovoltaics and gallium oxide power electronics. He has co-authored over 130 papers in peer-reviewed international journals and conferences.

Abstract: 17

Edge-Rich 2D Nanomaterials: Controllable Synthesis and Electrocatalytic Applications

Shaijumon

shaiju@iisertvm.ac.in

Abstract: 18

Magnetic flatlands

Subhadeep Dutta

sspsdd@iacs.res.in

Abstract: 19

Interfacial and topological superconductivity in 2D materials revealed by spin-resolved scanning tunneling spectroscopy

Sujit Manna

Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India

Topological insulators (TI) and interfacial superconductors (SC) are both topics of intense current interest in modern condensed matter physics. The combination of topological insulators and superconductors is expected to reveal novel physics. Iron-chalcogenide based superconductor have set a new paradigm in exploring microscopic mechanism of unconventional superconductivity and a race to discover high-T_c interfacial superconductor. It also offers a new platform to realize pristine topological superconductivity and Majorana bound state at relatively high temperature.

In this talk, I will show that a combined molecular beam epitaxy and spin polarized scanning tunneling microscopy (MBE-SPSTM) system is very powerful and unique tools for engineering low-dimensional quantum materials down to atomic scale. I will discuss our recent findings of atomic scale spin structure and superconductivity in single layer Fe-chalcogenide ($FeSe_xTe_{1-x}$) films grown on Bi-based 3D topological insulator. We show the existence of non-collinear antiferromagnetic state in a monolayer FeTe under 2D limit. A detailed investigation of the temperature, magnetic field and spatial evolution of the electronic structure across the magnetic domains indicates that the unit-cell of FeTe is in very close proximity to a superconducting phase transition that coexisting with the long-range anti-ferromagnetism. This will followed by discussion in the evidence for nematic electronic states in single layer $FeSe_{0.5}Te_{0.5}$ revealed by quasi-particle interference map, which provides an ideal platform to study novel emergent phase in close proximity to a topological insulator [1-3].

Finally, I will discuss a unique scalable approach towards building one-dimensional topological superconductor where strong interplay between superconductivity, spin-orbit coupling (SOC) and Zeeman field, laid the foundation to realize Majorana bound states [4].

References:

1. S. Manna, A. Kamlapure, L. Cornils, T. Hänke, E. M. J. Hedegaard, M. Bremholm, B. B. Iversen, Ph. Hofmann, J. Wiebe and R. Wiesendanger, Nature Communication 8 (2017) 14074.
2. T. Hänke, U R Singh, L. Cornils, S. Manna, A.Kamlapur E. M. J. Hedegaard, M. Bremholm, B. B. Iversen, Ph. Hofmann, J. Hu, Z. Mao, J. Wiebe and R. Wiesendanger, Nature Communication 8 (2017) 13939.
3. A. Kamlapure, S. Manna, L. Cornils, T. Hänke, M. Bremholm, B. B. Iversen, Ph. Hofmann, J. Wiebe and R. Wiesendanger, Physical Review B 95 (2017)104509.
4. P. Wei, S. Manna, M. Eich, P. A. Lee, and J. Moodera, Phys. Rev. Lett. 122 (2019) 247002.

Abstract: 20

Two Dimensional Heterostructures in Catalysis & Devices

T. N. Narayanan

Tata Institute of Fundamental Research - Hyderabad.
tnn@tifrh.res.in

Atomic layers based heterostructures are highly intriguing due to their interface induced properties. During the talk, a few such heterostructures will be discussed for their heterogeneous catalytic applications as well as photodetector developments. Some of the heterostructures such as graphene/hBN and graphene/MoS_2 are found to be active towards hydrogen evolution reaction, while their individual layers are not. A multi-scale modeling approach is undertaken to understand the interface induced catalytic phenomenon from these interfaces and an effect called 'van der Waals shadow effect' is unraveled. Such a hetero-structure catalyst, where graphene sits on the top, can also address the issues related to the stability of the transition metal dichalcogenides while using in electrocatalytic applications. Secondly, an approach towards the synthesis of catalyst free grown fluorographene (FG), a graphene derivative, will be discussed along with a photodetector development based on FG and a few layer MoS_2. The device performance show that such a heterostructure is advantageous over MoS_2 - Field Effect Transistor based photodetectors. Further, the results also promise the role of FG both as an active layer in the FET and dielectric medium.

References:

1. Hydrogen Evolution Reaction Activity of Graphene-MoS2 van der Waals Heterostructures, Ravi Biroju, Deya Das, Rahul Sharma, Shubhadeep Pal, Mawlong Larionette P L, Kapil Bhorkar, P K Giri, Abhishek Singh, and T. N. Narayanan, ACS Energy Letters 2, 1355–1361 (2017).
2. Stacking Sequence Dependent Photo-Electrocatalytic Performance of CVD Grown MoS2/Graphene van der Waals Solids, Ravi K. Biroju, Shubhadeep Pal, Rahul Sharma, P. K. Giri, and T. N. Narayanan, Nanotechnology 28 (8), 085101 (2017).
3. Mechanistic Insight in to Enhanced Hydrogen Evolution Reaction Activity of Ultra-Thin h-BN Modified Pt Electrodes, Anku Guha, Thazhe Veettil Vineesh, Archana Sekar, Sreekanth Narayanaru, Mihir Sahoo, Saroj Nayak, Sudip Chakraborty, and T. N. Narayanan, ACS Catalysis 8, 6636-6644 (2018).
4. On the Hydrogen Evolution Reaction Activity of Graphene-hBN van der Waals Heterostructures, Sumit Bawari, Nisheal M. Kaley, Shubhadeep Pal, Vineesh T V, Shamasree Ghosh, Jagannath Mondal, and T. N. Narayanan, Physical Chemistry Chemical Physics 20, 15007-15014 (2018).
5. Atomistic Elucidation of Sorption Processes in Hydrogen Evolution Reaction on a van der Waals Heterostructure, Sumit Bawari, T. N. Narayanan*, and Jagannath Mondal, The Journal of Physical Chemistry C 122 (18), pp 10034–10041 (2018).
6. Vapor Transport Deposition of Fluorographene Oxide Films and Electro-Optical Device Applications, Rahul Sharma, Ravi K. Biroju, Ofer Sinai, Hagai Cohen, Krishna Rani Sahoo, Vlada Artel, Hadas Alon, Adi Levi, A. Subrahmanyam, Wolfgang Theis, Doron Naveh, and T. N. Narayanan*, Applied Materials Today 13, 387-395 (2018).

Abstract: 21

Metal-chalcogen bond-length induced electronic phase transition from semiconductor to topological semimetal in ZrX2 (X = Se and Te)

S. Thirupathaiah *et al*[1]

S. N. Bose National Centre for Basic Sciences, JD Block, Sector 3, Slat Lake, Kolkata, 700106.

Tunable band gaps in layered TMDCs is one of the major research topics in recent days from both the theory and experiment. It is known that the band gaps in IVB TMDCs (TiX2, ZrX2, and HfX2, where X = S, Se, and Te) increase with the strain. However, among the IVB TMDCs, ZrX2 compounds in their monolayer thickness show peculiarity beyond a critical pressure. That means, instead of an increase in the band gap with the pressure, it starts decreasing with increasing the pressure. On the other hand, the monolayer thickness ZrTe2 transforms from metallic to a semiconductor beyond a critical pressure. Hence, understanding the pressure effects on electronic structure of TMDCs has a significance in their band engineering.

In this talk, I present the electronic structure of bulk ZrSe2 and ZrTe2 using angle resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) calculations. Our ARPES studies on ZrTe2 demonstrate free charge carriers at the Fermi level, which is further confirmed by the DFT calculations. An equal number of hole and electron carrier density estimated from the ARPES data, points ZrTe2 to a semimetal. The DFT calculations further suggest a band inversion between Te *p* and Zr *d* states at the Γ point, hinting at the non-trivial band topology of ZrTe2. Also, a comparative band structure study is done on ZrSe2 which shows a semiconducting nature of the electronic structure with an indirect band gap of 0.9 eV between Γ *(A)* and *M (L)* high symmetry points. We further notice that the metal-chalcogen bond-length plays a critical role in the electronic phase transition from semiconductor to a topological semimetal ingoing from ZrSe2 to ZrTe2.

1. I. Kar, Joydeep Chatterjee, Luminita Harnagea, Y. Kushnirenko, A. V. Fedorov, Deepika Shrivastava, B. Büchner, P. Mahadevan, S. Thirupathaiah, arXiv:**1907.03987**v1