2-Dimensional layered Quantum Materials: From Growth to Opto-electronic Transport

*Bubunu Biswal, Ramesh Rajarapu, Prahald Kanti Barman, Renu Yadav, Saroj Poudyal, Abhishek Misra**

Centre for 2D Materials research and Innovations, Department of Physics Indian Institute of Technology Madras, Chennai, India. 600036

CTQM2022

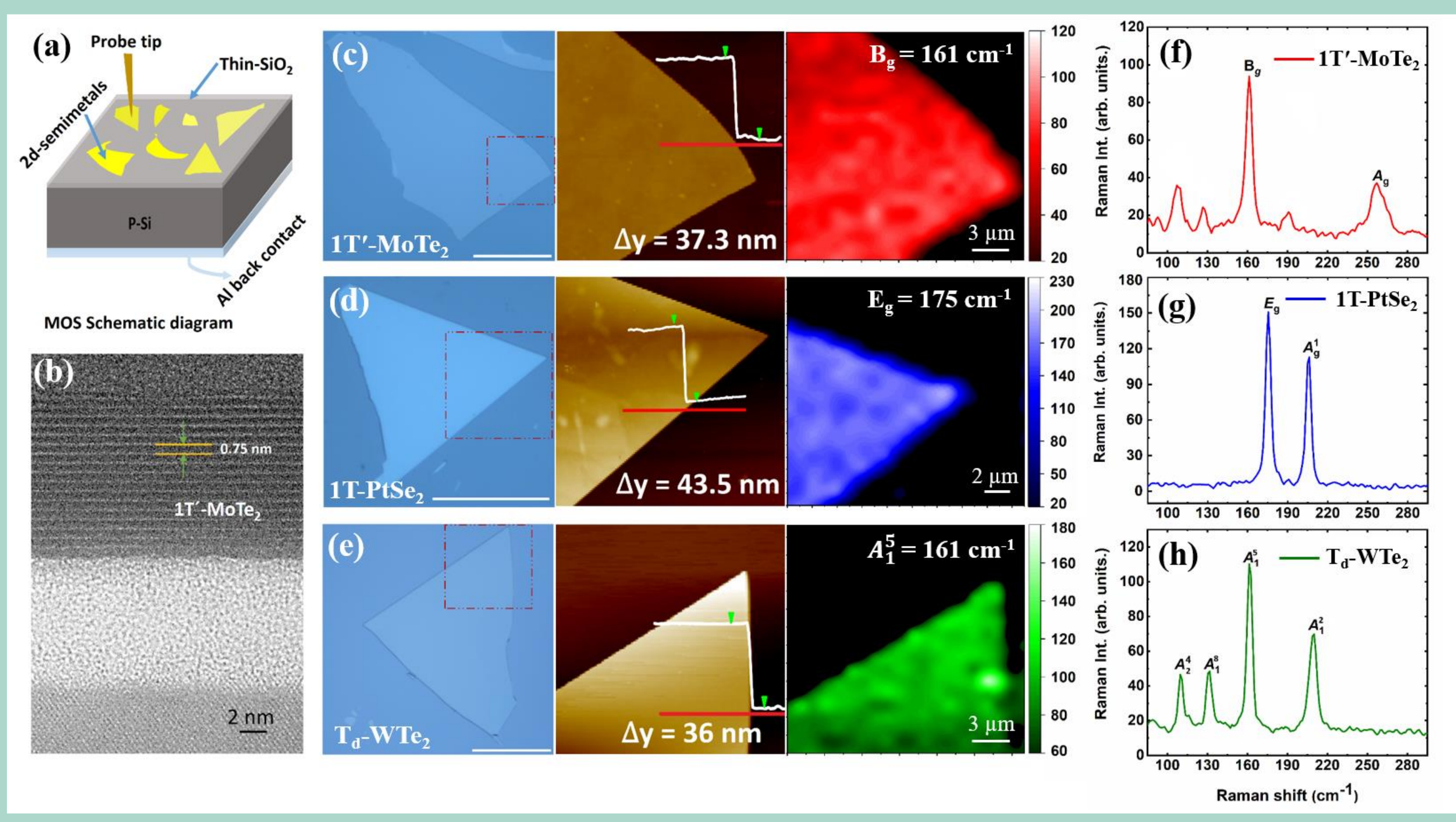
Highlights

Topological Semimetals | **R-phase Semiconductors**

Abstract- Layered 2-dimensional (2D) transition metal dichalcogenides (TMDCs), through different polymorphic phases and broad range of bandgaps, provide a rich landscape to study range of physical phenomena occurring at atomically thin dimensions. In order to access the novel topological nontrivial phases through quantum transport measurements, it is inevitable to have high quality materials of semiconducting and metallic nature and make high quality electrical contacts. Among the 2D TMDCs, 1T-$PtSe_2$, 1T′-$MoTe_2$, T_d-WTe_2 etc. show semimetallic behaviour and can be used as electrodes forming high quality, smooth, dangling bond free interface with 2D semiconductor channel. For a metallic electrode, its work function is a crucial parameter to decide the carrier flow across the interface. In this direction, we have evaluated the work function of 1T-$PtSe_2$, 1T′-$MoTe_2$, T_d-WTe_2 using the metal-oxide-semiconductor capacitor device structures. For semiconductors, we have developed a novel phase selective growth methodology to grow rhombohedral(R)-phase MoS_2 having sword like geometry with lengths up to 100 µm and uniform width and thickness. The grown MoS_2 shows good electrical properties with a mobility of 40 cm^2/V-s, I_{on}/I_{off} ratio of ~10^6 and high value of degree of circular polarization ~58% at 100 K temperature. The second harmonic spectroscopy shows the non-linearity of the R-phase irrespective of even and odd number of layers which is in contrast to H-phase MoS_2. These findings are significant for the development of future quantum devices based on ultrathin layered materials.

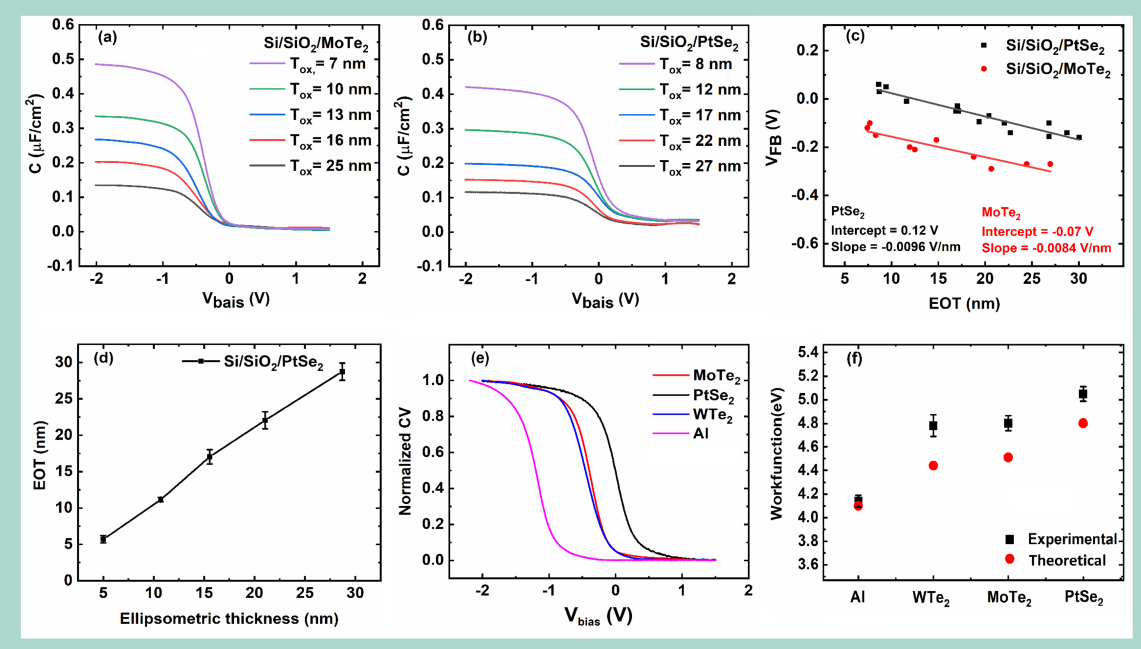
Work Function of semimetals

- Test Structure : Metal-Oxide-Semiconductor capacitor



- The 2D semimetals are exfoliated onto the thermally grown Si/SiO_2 substrate to fabricate the MOS device structure.
- The cross-sectional TEM image showing the clean semimetal/SiO_2 interface.
- The AFM image showing the thickness of semimetal, Raman spectrum and the Raman mapping of the MOS devices certify the semimetals used.
- The exfoliated flakes were directly probed using the tip of the probe station.

Capacitance Voltage (CV) Analysis

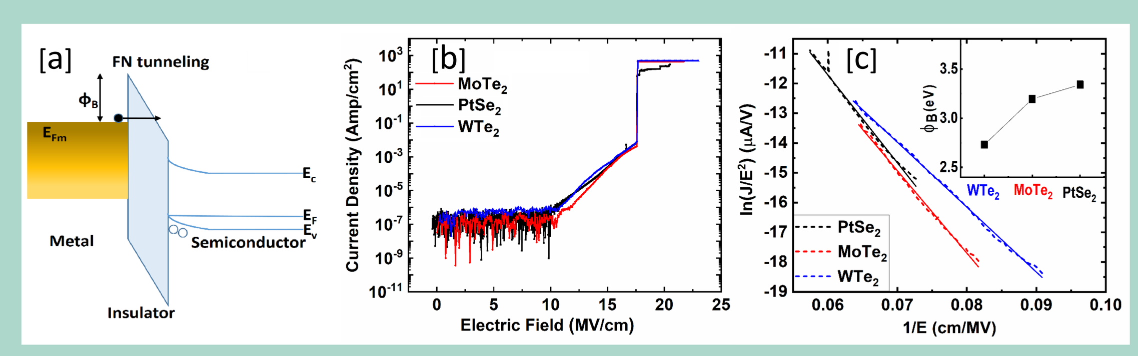


- All the CV irrespective of the semimetal are well shaped, which confirms the good quality of oxide and the semimetallic electrode.
- The flatband voltage extracted over different thickness gives the contribution of the oxide charges to its shift.

$$V_{FB} = \Phi_{ms} - \frac{Q_f + Q_{it}}{C_{max}}$$

- The work function estimated using our experiment are in a good agreement with the DFT calculated value.

Current Voltage (IV) Analysis



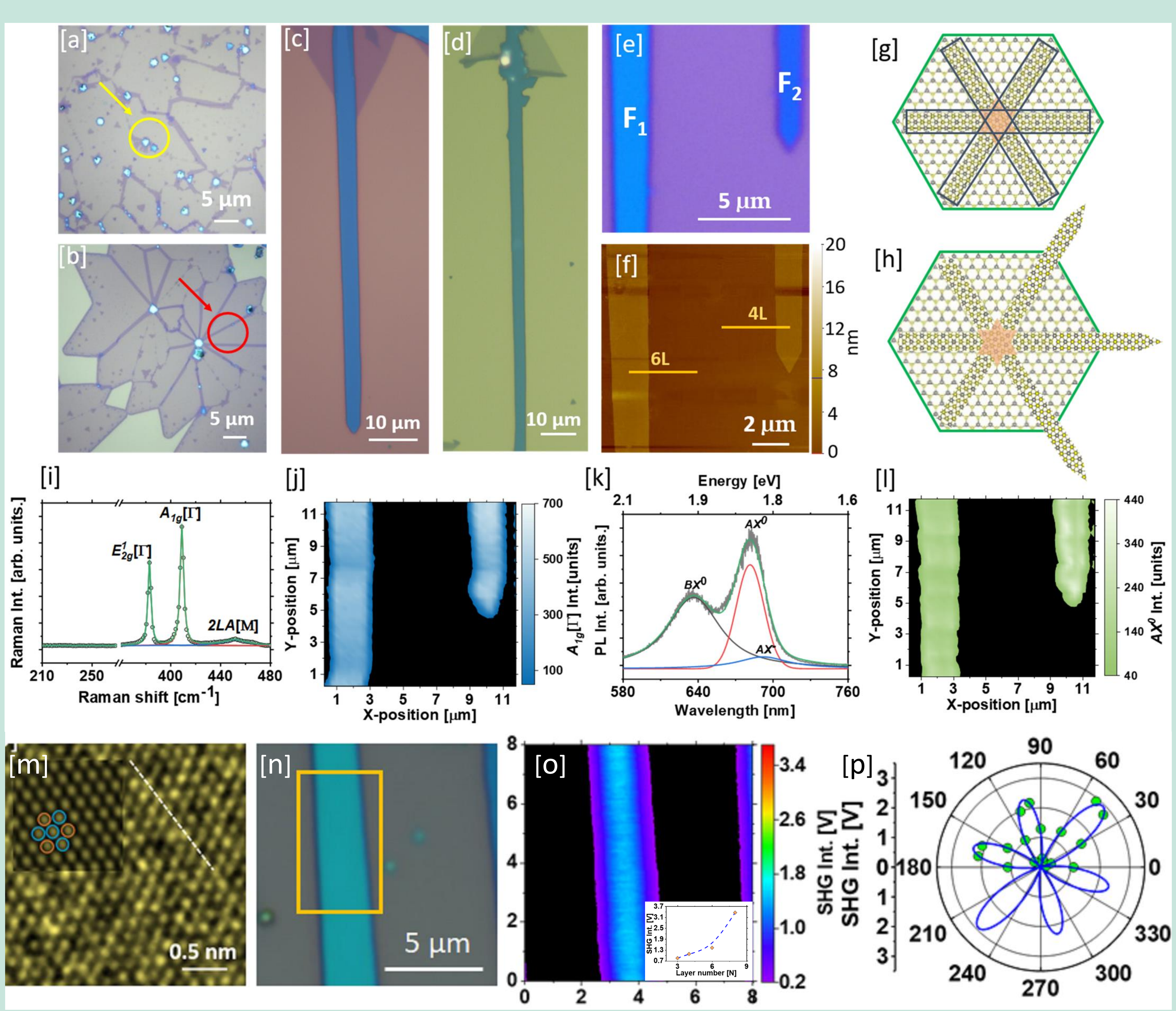
- The breakdown study of MOSCAPs have been done in accumulation mode.
- The barrier heights extracted from the IV analysis by fitting the FN tunnel current regime is also following the same trend of the work function value.

Ref -: Appl. Phys. Lett. ***120****, 093101 (2022)*

Rhombohedral (R-phase) MoS_2

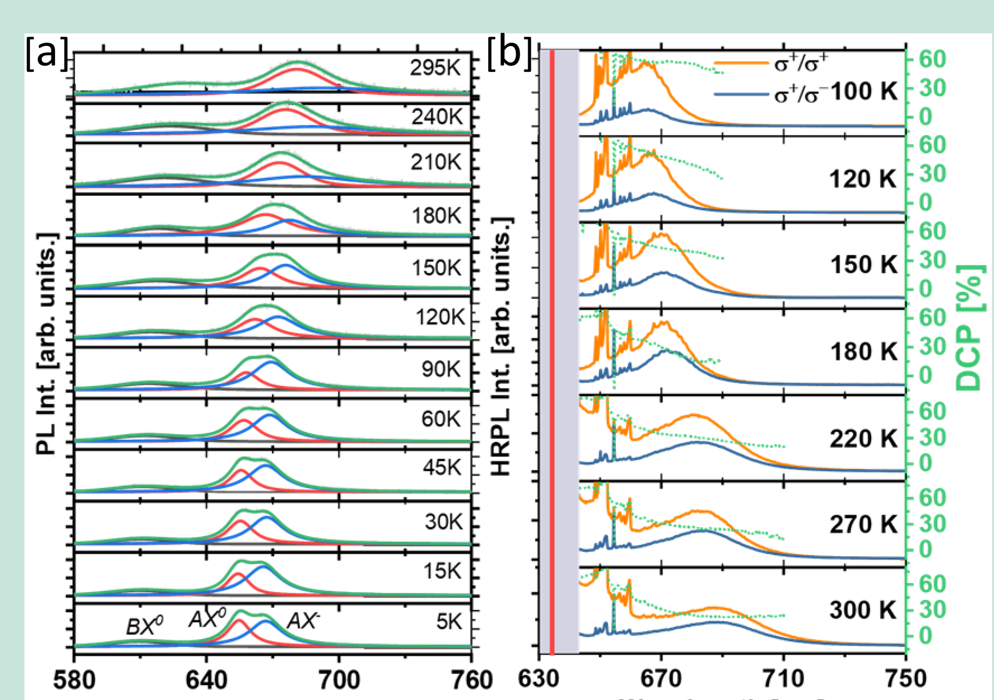
Key Significance -:

- ❑ *Broken Inversion symmetry,*
- ❑ *Layer independent second harmonic generation,*
- ❑ *High valley polarization.*



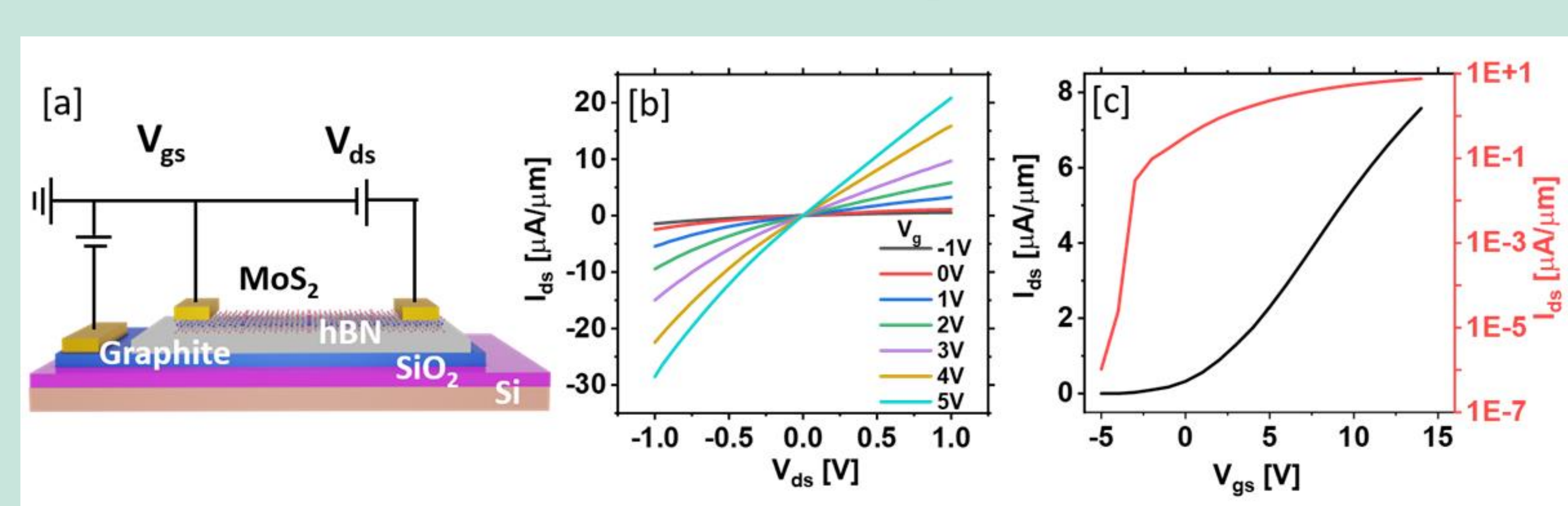
- The MoS_2 long strips (~100 µm) with a variable thickness (3L to 8L) have been grown by pulsed-CVD method.
- The as grown high quality MoS_2 strips has uniform width and thickness along the length of the strip.
- MoS_2 strips are of R-phase having exciton peak separation (AX^0 & BX^0) of ~ 140 meV.
- R-phase stacking arrangements of layers are confirmed by HRTEM measurements.
- SHG intensity throughout the strip irrespective of even or odd number of layer confirms the inversion symmetry breaking the in the R-phase MoS_2 in contrast to H-phase MoS_2.

Evolution of trion peak & High valley polarization of (R-phase) MoS_2



- Evolution of exciton (AX^0) and trion (AX^-) as function of temperature. Below 200K, existence of trion is more prominent and dominating too.
- Energy separation of exciton and trion is ~ 34 meV at 5K.
- Valley polarization of 6L R-MoS_2 is ~ 58% at ~ 100K.
- High degree of valley polarization is achieved even in few layer thick MoS_2 as the inversion symmetry breaks in R-phase, where consecutive 2L are of AB stacking configuration.

Electrical characterization of R-phase MoS_2 strip



- We have fabricated the graphite back gated transistor with R-phase MoS_2 strips as channel material.
- The linear and symmetric characteristic for small bias voltages indicated good Ohmic contact between the R-MoS_2 channel and Ni/Au source and drain electrodes.
- Transfer characteristics showed an I_{on}/I_{off} of 10^6 with mobility of 40 cm^2/V-sec and SS of 309 mV/dec.
- Contact resistance of 2.5 kΩ-µm was calculated using Y-function method.

Conclusions

- We have estimated the work function of the 2D semimetals, which enable us to choose them as electrode to the layered channel material to access the barrier free transport.
- Our group have grown the high quality R-phase MoS_2 with better optical and electrical transport properties.
- We are working on the growth and physical properties of 2D materials for energy efficient, high performance, multifunctional quantum electronic devices.

Acknowledgements- Dept. of Physics and CNNP, Dept. of EE, IIT Madras, Chennai, India.

Email - abhishek.misra@iitm.ac.in