Title:	Exploring the Interfacial Properties of two-Dimensional Materials and Van Der Waals Heterostructures
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Abstract:	Two-dimensional (2D) materials and their van der Waals heterostructures are viable candidates for futuristic nanoelectronics devices owing to their astonishing electronic, and optical properties. To advance the application of electronic devices based on 2D layered materials, it is essential to understand the fundamentals of electronic energy band alignment and charge transfer at the contacts and interfaces. So far band alignment at the contacts has traditionally been estimated analytically by following various transport models or measured indirectly from electronic response. However no direct experimental protocol was established so far to measure the crucial interface parameters at real condition of a contact/interface and estimate the deviation of these factors with ideal conditions. Thanks to 2D materials which can create a clear distinct, uniformly abrupt and non-diffusive interface (unlike bulk contacts) and enables us to probe the electrostatics at the nanoscale level exactly at the interface. We approached the Kelvin Probe Force Microscopy (KPFM) technique, an Atomic Force Microscopy (AFM) based advanced tool to probe the surface potential, to understand the electronic band alignments at the contact metal/2D interfaces as well as at the van der Waals heterostructures interfaces and applied the semi-classical electrostatic tactics to deduce interface parameters. For such nanoscopic measurements to investigate the spatial distribution of surface potential, MoS 2 is an appropriate candidate since it is a stable 2D semiconductor with high carrier mobility. Furthermore, we also examined the twisted MoS 2 /MoS 2 homo-interface with hexagon morphology using room temperature μ-PL(Photoluminescence) which could be useful in the field of electronic devices based on twistronics. In addition to the band alignment at interfaces, we have experiences that MoS 2 's morphological shape can also modify its band structure. We employed low-temperature μ-PL to examine the influence of morphological shape on the optoelectronic properties of MoS 2 . My first work focuses on the probing of energy band bending at the Au/ MoS 2 junction during current conduction in a bridge-type MoS 2 channel. MoS 2 flake was transferred on pre- fabricated Au electrodes to avoid the contamination caused by chemicals used in the lithography process. A thorough investigation of the surface potential during charge transportation revealed asymmetric contacts between MoS 2 and Source contact and Drain contact as well as Schottky behaviour at the MoS 2 /Au interface. By varying the applied bias to MoS 2 channel, we have determined the interface parameters like built-in potential, surface ielectric field, and space charge density at Au/MoS 2 interface in non-equilibrium conditions. The experimentally determined depletion width is compared with analytically calculated depletion width and the difference between both attributes to local defects, contact area, and thickness variation of MoS 2 flake. The interface parameters and their variation with the current conduction can all be probed, opening the door to comparing and improving the performance of real devices against ideal ones. In second project, we have probed the surface potential at the MoS 2 /BP van der Waals p-n heterojunction constructed by the dry transfer method. By using the Kelvin probe force microscopy (KPFM) technique to measure the spatial distribution of built-in potential, built-in electric field, and depletion width, we are able to demonstrate the formation of the p-n junction at the MoS 2 /Black phosphorene (BP) interface and experimentally measure the band alignment under realistic circumstances . We have optimised the lift height of ~15 nm to get better resolved potential image. By changing the thickness of the MoS 2 flakes over a uniform thickness of BP flakes, the charge distribution at the MoS 2 /BP interface has been modulated. The increase in the lateral built-in potential and lateral built-in electric field at MoS 2 /BP interface is observed with increasing the thickness of the MoS 2 flake. Moreover, the Density Functional Theory (DFT) calculations have been done to validate the experimental findings. In the third project, we examined the twistronic of CVD-grown MoS 2 /MoS 2 interface with hexagon morphology. We performed room temperature PL measurements and found the blue shift in the PL peak position at the interface. The shift in the PL energy attributes to the lattice strain induced by the angular shift between two flakes. We have measured the angle between two flakes with FESEM which is found to be 6.7 degrees. Deconvoluted PL spectra revealed unequal shift in the peak energy of A exciton, B exciton and trion at the MoS 2 /MoS 2 interface. The energy shift in B exciton at the MoS 2 /MoS 2 interface is more prominent. We observed an increment of ~19 meV in the valence band splitting energy at the interface. In addition, the optical properties of MoS 2 with a morphological hexagon shape have been explored in the fourth project. The Chemical Vapor Deposition (CVD) technique was used to synthesize the hexagon morphological shape of multilayer MoS 2 flake. Temperature-dependent PL studies reveal the red shift in PL owing to change in band gap due to semiconducting properties. Deconvoluted PL spectra demonstrate the change in PL intensity as well as PL red shift of trions, A exciton and B exciton. Variation in ratio of A exciton intensity to B exciton iiintensity with the temperature aids to calculate the fermi energy ~ 31 meV at room temperature which is quite low. High electron concentration of order ~ 1.5×10 12 cm -2 has been determined regardless of multilayer nature of MoS 2 hexagon. We observed enhancement in electron phonon coupling in the case of MoS 2 in hexagon morphology. The fitting parameters to change in PL peak energy with temperature determines the band gap~1.91 eV at absolute temperature which is high as compared to previous reports (~1.8 eV) for other morphological shapes. From line width variation with temperature, we are able to determine the exciton-optical phonon coupling strength. The valence band splitting energy is determined to be ~132 meV which doesn't vary significantly with the temperature.
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