Abstract

The journey of 2D materials begins with the isolation of graphene in 2004 at the University of Manchester. The properties of these low dimensional materials can precisely be controlled due to the quantum confinement effect. In 2D materials, different layers are held together by strong in-plane interaction and weak out-of-plane bonding, allowing isolation of individual layers and mixing them with other materials. Recently, the van der Waals (vdW) heterostructures obtained by stacking different layered materials with other materials have drawn huge attention due to their unique electronic properties. These heterostructures are the basis of today's digital electronics with enormous computational power packed into a smaller space. Therefore, in this thesis work, we have extensively studied the exciting physics of 2D/3D heterostructures.

Band alignment across these heterostructures do play a surprisingly strong role for modeling electronic and optoelectronic devices for their specific applications. Before using a heterostructure for a particular application, it is an absolute necessity to find its band alignment. Thus, in this thesis work, before exploring the particular applications of MoS_2/Si and MoS_2/GaN heterostructures, we have studied the band alignments at the heterointerfaces. We have measured the conduction and valance band offsets across the 2D/3D heterojunctions by using X-ray and Ultraviolet photoelectron spectroscopy techniques. Interestingly, we obtained a type-I and type-II band alignment across the MoS_2/GaN and MoS_2/Si heterojunction, respectively, which is particularly useful for designing optoelectronic devices. Due to the conducive band alignments, we have demonstrated the photo-sensing applications of both the heterostructures. Moreover, the photo-sensing behavior strongly depends on photoinduced charge transport across the heterointerface. Based on the measured position of Fermi level used in the band alignment process at the heterointerface, we have identified the movement of charge carriers at the heterojunctions. In MoS_2/Si heterostructure, we have also given an insight into different scattering mechanisms influencing the carrier dynamics at the heterostructure. Here we observe that absorption of single-photon may result in the generation of multiple charge carriers, confirming the suitability of MoS_2/Si heterostructure for high-efficiency optoelectronic devices. Our fabricated optical sensor demonstrated a very high photoresponsivity and specific detectivity, making it a perfect candidate for sensing even a very small optical signal in the visible range.

MoS_2/Si heterostructure based photodetectors possess a wide spectral response ranging from ultraviolet to near-infrared region. However, in the UV region, the MoS_2/Si photodetector showed poor performance. Hence, by using GaN as a wide bandgap semiconducting material in MoS_2/GaN heterojunction, a very high value of absorbance in the UV range could easily be obtained. In this thesis work, we have achieved a spectral responsivity of the order of 3, which is not possible to be obtained by only GaN-based or only MoS_2-based optical sensors. By forming the heterojunction, we have leveraged the advantages of both the constituent semiconductors. We have achieved a response time of 5 ms, which is significantly better than the earlier MoS_2 based photo-sensors. The response time can further be reduced by reducing the active area of the device. A reduction in the area will reduce the RC constant of the photo-sensor and makes the device ultrafast. UV photo-sensors have a wide range of applications in the field of environmental protection, medical science, defense security, and remote control.

Today we are living in the era of multifunctional devices. A single functional device cannot be used for advanced technological applications. In this thesis work, to check the suitability of our device for multifunctional operations, we have evaluated the gas sensing performance of MoS_2/GaN based heterostructure. Our obtained results exposed the potential of MoS_2/GaN heterojunction based gas sensors for ultrahigh sensitivity and quick detection of hydrogen gas molecules at a very low operating power. Generally, the sensitivity, selectivity,

recovery, and response time are the key parameters to evaluate the performance of practical gas sensors. The available large surface area provided by the 2D MoS_2 thin-film facilitates more number of active sites for the hydrogen to get adsorbed. Besides, the MoS_2/GaN junction offers a barrier at the interface for the movement of charge carriers. Upon hydrogen exposure, the molecular adsorption tuned the barrier height at the MoS_2/GaN interface under the reverse biased condition, thus resulting in high sensitivity. Our results reveal that temperature strongly affects the sensitivity of the device, and it increases from 21% to 157% for 1% hydrogen with an increase in temperature (25-150 °C). The sensing mechanism was demonstrated based on the energy band diagram at the MoS_2/GaN interface in the presence and absence of hydrogen exposure. Therefore, a single device could be used for UV detection and gas sensing applications confirming its multifunctionality. The proposed methodology can readily be applied to other combinations of heterostructures for sensing different gas analytes. Moreover, the device performance strongly depends on many external factors, and temperature is one of the most crucial factors among them. Therefore, in the last part of this thesis work, we have studied the carrier transport across the heterointerface under thermal excitation. Our results reveal that temperature vigorously affects the interfacial parameters of the device.

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