

Since the isolation of graphene in 2004 by Geim and Novoselov, two-dimensional (2D) materials have been opened new avenues for developing next-generation electronics devices. 2D semiconducting MoS₂ with a tunable bandgap, being the frontrunner of layered transition metal dichalcogenides (TMDCs) family has grabbed the renewed interest of the research community by providing unprecedented device performance at the atomic scale. This thesis work is focused on most vibrant gas and light sensing applications of chemical vapor deposition (CVD) grown 2D MoS₂.

Different nanostructures including horizontal flakes, vertical flakes and nanowires network of the MoS₂ were synthesized by using the CVD process and examined their gas sensing characteristics to explore the role of different adsorption sites of MoS₂. It was observed that edge sites of MoS₂ exhibit higher gas adsorption compared to that of terrace sites on the basal plane of MoS₂ because edge sites have a large number of dangling bonds as well as high d-orbital electron density. In this context, the MoS₂ nanowires sensor with high edge sites-to-volume ratio exhibited better sensitivity with detection limit to 4.2 ppb NO₂ as compared to that of horizontal and vertical aligned MoS₂. Further, defect and interface engineering were simultaneously utilized for improving the gas sensing performance of the MoS₂ sensor. Optimal sulfur vacancies as defects were deliberately created in vertically aligned MoS₂ via thermal annealing and then, rGO nanoparticles were loaded on the sulfur vacancy containing MoS₂ (Sv-MoS₂) for forming rGO/Sv-MoS₂ heterojunctions. P-type rGO changed the intrinsic n-type semiconducting behaviour of MoS₂ into p-type via enhancing charge transfer through chemical bonding in between rGO and Sv-MoS₂. As a result, p-type rGO/Sv-MoS₂ sensor exhibited excellent sensitivity to NO₂ with complete recovery at low temperature (50 °C) by exploiting electronic and chemical sensitization.

Despite the high sensitivity to NO₂ gas at room temperature, slow response and incomplete recovery restrict MoS₂ usage on a commercial gas sensing platform. To address slow response/recovery kinetics, MoS₂ gas sensor was tested under thermal and optical energy sources. The temperature was capable to achieve full recovery with the expense of sensitivity, however, the sensor showed enhanced sensitivity with complete recovery at room temperature under UV light irradiation. In addition, nucleation controlled one-step CVD process to synthesize MoS₂-MoO₃ hybrid micro flowers using vapor transport process was developed. The MoS₂-MoO₃ hybrid sensor showed good response to NO₂ gas with complete recovery at room temperature without using any extra energy source (temperature or UV light). This research work helps to remove the microheater from commercial metal-oxide gas sensor technology due to gas detection at room temperature.

In the last part of the thesis, 2D MoS₂ is also explored in optoelectronics application via fabricating a photodetector using a van der Waals heterostructure of the MoS₂ and rGO. This vertical out-of-plane rGO/MoS₂ heterojunctions exhibited high responsivity and detectivity in visible range wavelengths with excellent stability in air ambient as a result of the synergistic effect of enhanced photoexcited carrier density and photogating effect. The potential challenges and future perspectives in the emerging MoS₂ research for sensing applications are also discussed.

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