ABSTRACT

Two-Dimensional (2D) Materials are crystalline materials consisting of a single layer of atoms with a thickness of a few nanometers or less. 2D- Transition metal dichalcogenide (TMDCs) are kind of 2D materials such as MoS_2, WSe_2, $MoTe_2$, etc. have a tunable bandgap and are being investigated experimentally and theoretically using density functional theory (DFT) calculations. DFT is a powerful theoretical tool to model the physical, electronic, and optical properties of 2D materials. In this thesis work, using DFT calculations, we systematically explore the possibility of band structure engineering of 2D monolayers by substitutional doping technique using different dopants belonging to 3d, 4d, and 5d groups of the periodic table. Transition metals (TM) are a popular choice of substitutional dopants in TMDCs material. Our results suggest that the **V, Nb, and Ta dopants** are only potential **p-type dopants**, and **Re is an n-type dopant** for the WSe_2 monolayer. In this work, we investigated the band structure, projected density of states (PDOS), and optical spectra of TM- doped 2D semiconductor monolayers such as **WSe_2, and Al-doped g-ZnO (g-AZO) modulated by biaxial strain**. We theoretically investigated the electronic structure and optical properties of Nb, Ta, and Re-doped WSe_2 monolayer by applying biaxial tensile and compressive strain. We also investigated the strain-dependent behaviour of formation energy (E_{form}) for Nb, Ta, V, and Re doped-WSe_2 monolayer using DFT calculations. Further, we systematically studied the strain-dependent doping behavior and optical absorption of the g-AZO monolayer under the application of strain (ε_{xy}) by using Hybrid-DFT calculations. It is observed that **Strain engineering** can be used to **enhance doping concentration** in 2D semiconductors which is useful in **optoelectronic device applications.**

The 2D materials-based heterostructures are highly explored by the device community due to their atomically thin nature, large surface area, and various degrees of freedom. The application of 2D heterostructure mainly depends upon the atomic commensurability, interlayer interaction, charge transfer between constituent 2D materials, and particularly band alignment when heterostructure is formed. Therefore, in this work, we systematically investigated the modulation of electronic structure and optical spectra of **GaTe/$MoTe_2$ van der Waals (vdWs) heterostructure** using Hybrid-DFT calculations. Currently, electronic devices based on these 2D TMDCs materials with Silicon are at the forefront of current research due to their potential applications as p-n junctions, solar cells, LEDs, photodetectors, and photovoltaic cells. A promising approach is to combine two high-performance materials to create a mixed-dimensional heterostructure that performs beyond existing technologies and enables very high sensitivity, low-cost production, and high photodetection gain. A fabricated **2D-0D-3D broadband photodetector** shows an excellent rectifying nature with a **good rectifying ratio and high photoresponse and fast transient time** with significant optoelectronics applications.