Abstract

Two-Dimensional (2D) Transition Metal Dichalcogenides (2D-TMDs) are promising materials for next-generation nano-electronic devices because of their interesting electronic properties ranging from metal to semiconductor to insulator to even topological insulator. The thesis is motivated by the recently realized both experimentally and theoretically, a new class of TMDs, known as Janus (W/Mo) SSe monolayer. The stability of Janus monolayers is studied using the phonon band structure. The strain is used to interplay the optoelectronic properties of Janus WSSe monolayer, and interestingly strain mediated electronic transitions are noticed. The tensile strain is relatively more sensitive as compared to that of compressive strain. Additionally, the controlled defects are explored in (Mo/W) SSe Janus monolayers. The vacancy defects showed non-magnetic characteristics together with the onset of magnetic ordering with some antisite defects. The chalcogen antisite and vacancy defects are the most stable among the various explored defects. The gas sensing characteristics are investigated on pristine MoSSe, WSSe, and the stable defect included monolayers as well for H_2S, NH_3, NO_2, and NO toxic gases. The pristine MoSSe and WSSe Janus monolayers showed relatively better gas sensing characteristics as compared to their parental MoS_2, $MoSe_2$, WS_2, WSe_2 chalcogenide monolayers. The selenium surface in Janus WSSe monolayer showed strong adsorption with respect to the sulfur surface. Further, the chalcogen vacancy led to improved gas sensing characteristics because of the availability of active sites. Thus, MoSSe and WSSe monolayers seem to be potential 2D materials for NO_2 and NO gas sensing applications.

The thesis work is extended to explore the optoelectronic properties of bulk WS_2, WSe_2 and the noticed very high absorption coefficient make them suitable absorber materials for solar cell applications. Moreover, the electronic and optical properties of WSSe and WSeTe monolayers are investigated, and the computed low absorption and high bandgap make them suitable buffer layers for $W(S/Se)_2$ absorbers. The single-junction photovoltaic performance is optimized for $W(S/Se)_2$ absorbers together with WSSe and WSeTe buffer layers. The effect of absorber layer thickness, carrier concentration, defect density, contact work function, and buffer layer thickness, carrier concentration, and interface defect density are investigated to understand the performance of solar cells. The maximum efficiencies of about ~ 17.73% and 18.87% are noticed for optimized single-junction WSSe/WS_2 and WSSe/WSe_2 solar cells. Further, the thermoelectric properties of WSSe monolayer are studied using the DFT together with semi-classical Boltzmann theory. We observed that the tensile strain reduces the lattice thermal conductivity from 25.37 to 9.90 $Wm^{-1}K^{-1}$. Further, the biaxial tensile and compressive strains mediated valley degeneracy led to the improvement in the power factor. As a consequence, the figure of merit is improved from 0.90 (0.74) to 1.25 (1.08) under biaxial strain for n(p) type carriers. Thus, the thesis work carried out on Janus TMDs monolayers will provide a framework for the experimentalist to design the nano-devices for various applications such as sensors, ultrathin solar cells, and thermoelectric devices.