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Conclusion and Future scope of work

The TMDs based monolayers exhibit wide range of electronic properties depending on the crystal symmetry and transition metal d-orbitals. The appropriate electronic properties and derivative quantities make them suitable for nano device applications. Recently, a new MoSSe monolayer is experimentally realized called the JTMDs. It has various advantages including the broken mirror symmetry and two different chalcogen atomic surfaces over the conventional TMDs monolayers. These additional properties of JTMDs monolayers make them promising candidate to explore these materials for various application such as piezoelectric, water splitting and valleytronics. Here, we have considered the three JTMDs monolayers, MoSSe, WSSe, and WSeTe monolayer and explored their uses in nano device applications, as summarized in Figure 8.1.

The dynamic stability of MoSSe, WSSe, and WSeTe monolayers is investigated using the phonon band structure. The electronic band structures of considered monolayers ensure the direct band gap. Janus WSSe monolayer confirms the large band gap compared to MoSSe. The maximum sustainable biaxial compressive and tensile strains are computed using the dynamic stability using the respective phonon band structures. The Janus WSSe monolayer is stable up to 8% tensile strain and up to 1% compressive strain only. The direct to indirect transition is observed against the biaxial compressive and tensile strained monolayers. The other electronic derivative quantities like effective mass and mobility are also explored on strained monolayers.

The electronic and magnetic properties of vacancy and antisite point defects included MoSSe and WSSe monolayers are studied. The chalcogen atom antisite site defects are most stable. These defects provide an active site for adsorption of toxic gases. The H_2S, NH_3, NO_2, and NO gas molecules are considered for adsorption. The pristine and point defects included MoSSe and WSSe monolayers are considered as the host for adsorption of gas molecules. Adsorption on pristine WSSe monolayer ensures the high sensitivity towards selenium surface. The computed recovery time confirms the fast recovery of gas molecules. The WSSe monolayer showed the higher sensitivity over the MoSSe monolayer. The antisite and vacancy defects exhibit enhanced gas sensing characteristics, and among these defects, vacancy defects exhibit relatively higher sensitivity.

The optoelectronic properties of bulk WS_2/WSe_2 materials are suitable for absorber materials in solar cell applications. The ultra-thin WSSe/WSeTe layers have low absorption coefficient and thus, suitable for buffer layers. The electronic and other properties are calculated from DFT required to simulate the performance of solar cell using SCAPS-1D microscopic simulation program. The PV performance is investigated by analysing efficiency η, short circuit current density Jsc, open circuit voltage Voc, and fill factor. The effect of thickness, carrier concentration, and carrier concentration of absorber and buffer layers is investigated to understand their impact on PV performance. The impact of minority charge carrier and interface recombination speed are considered for simulating more realistic PV devices. Considering these effects, we optimized the device parameters and the maximum possible efficiency of solar cells is predicted.

The thermoelectric properties of WSSe monolayer are studied in terms of Seebeck coefficient, electrical conductivity, thermal conductivity, power factor, and figure of merit of Janus WSSe monolayer. The lattice thermal conductivity is continuously decreasing with increasing temperature. The biaxial compressive and tensile strains driven thermoelectric properties are investigated. The biaxial strain leads to valley degeneracy in VB and CBs, which enhance the electrical conductivity and Seebeck coefficient. The tensile strain is relatively advantageous in reducing the lattice thermal conductivity, and thus, improving the thermoelectric properties. The strained monolayer showed improvement of ~ 29% thermoelectric device efficiency with respect to that of the unstrained monolayer.

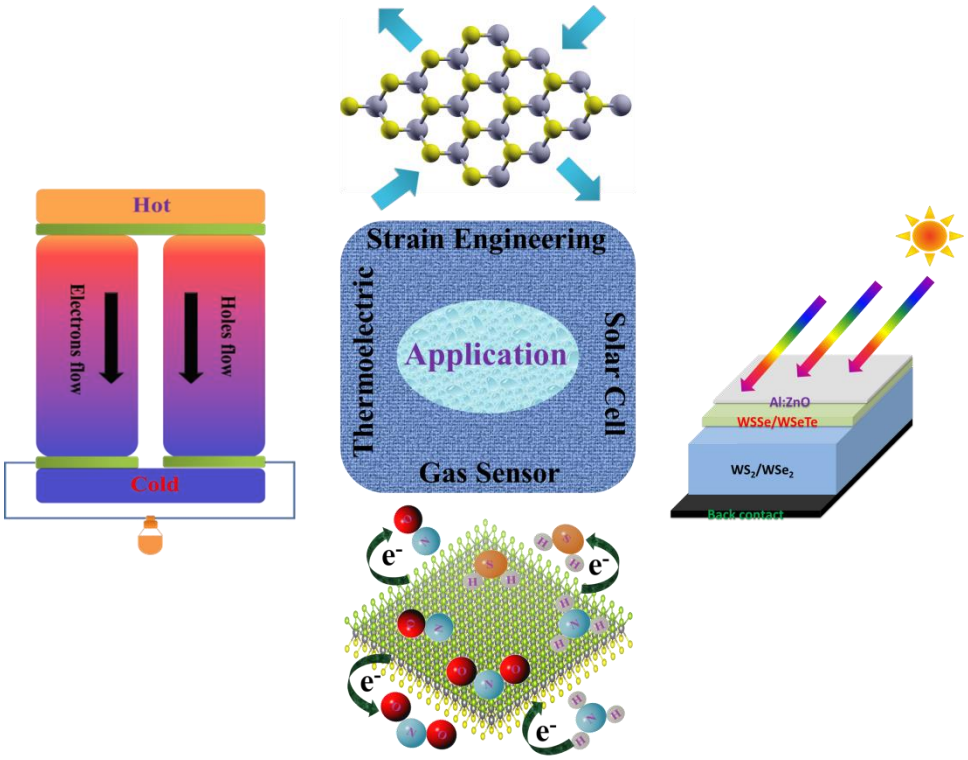

Figure 8.1 Explored applications of Janus monolayers

Thus, in brief the thesis work covered the detailed study about of structural stability, electronic and optical properties of Janus monolayers together with strain and defect engineering. These monolayers are explored for various applications like, gas sensor, solar cell and thermoelectric devices.

The JTMDs monolayers have ultralow thickness, very high surface to volume ratio, and excellent electrochemical properties, providing more active sites for ions for energy storage applications. The electrodes based on JTMDs may be the best choice for energy storage applications. The pristine JMTDs monolayers exhibit exceptional electronic properties for semiconductor devices. In addition, the strain dependent structural and electronic properties suggest that these materials may be the best choice for flexible electronic device applications, which can protect the degradation of electronic devices because of the large strain tolerance. The high absorption coefficient and mobility with suitable bandgap of these monolayers may also be suitable for photodetector applications in respective energy ranges. Thus, there is enormous potential for these JMTDs based monolayers for not only in terms of understanding the materials physics but also for next generation electronic devices, as summarized schematically in Figure 8.2.

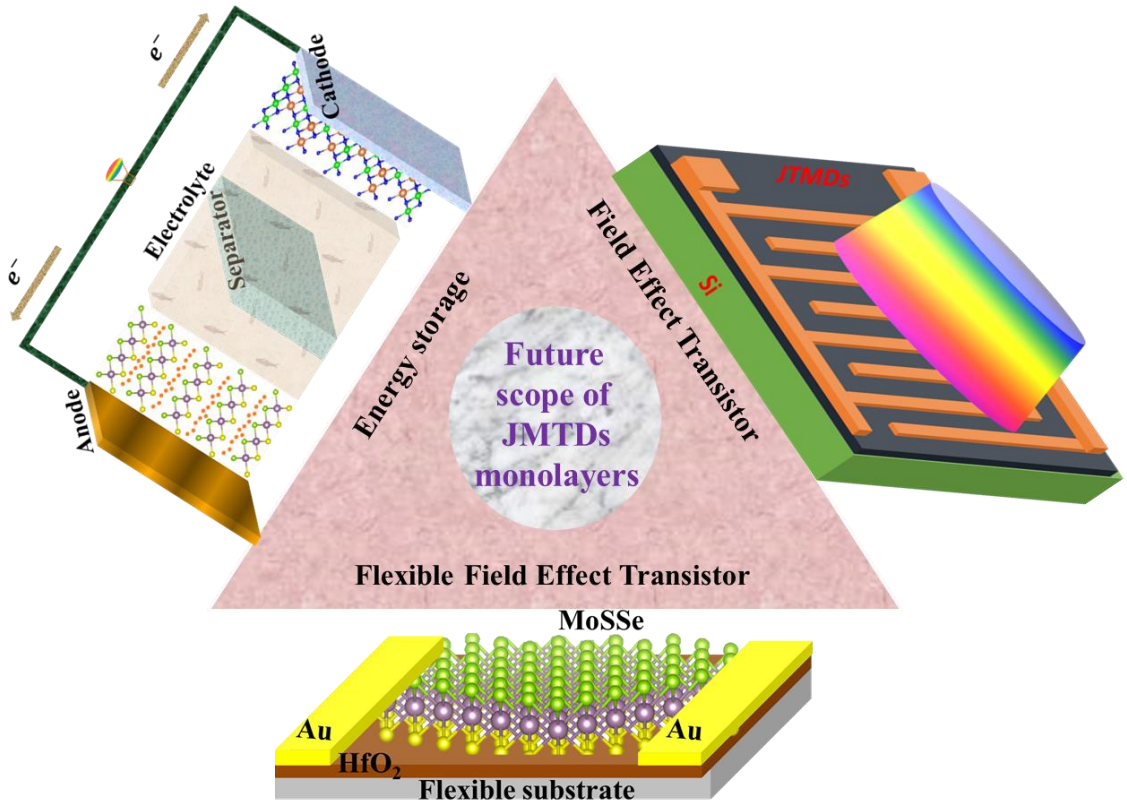

Figure 8.2 The potential future possibilities with Janus monolayers

The more interesting aspect is the inherent breaking of inversion symmetry in these monolayers, which induce ferroelectric and piezoelectric characteristics intrinsically. Further, the controlled defects in these monolayers may induce magnetic ordering and thus, novel ultrathin multiferroic systems can be designed and developed. These materials will be very suitable for realizing multistate memory devices. The integration of these materials with existing electronic materials and devices can be explored to harness the various potentials applications of such monolayers.