Title:	2D TRANSITION-METAL DICHALCOGENIDE MONOLAYERS AND THEIR JANUS STRUCTURES FOR NEXT-GENERATION ELECTRONICS AND ENERGY CONVERSION: AN AB-INITIO STUDY
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Abstract:	The interplay of charge, spin, and valley pseudospin degrees of freedom (DOF) in a single integrated system is the future prospect of next-generation electronic devices. In this thesis, monolayers (ML) of Group-VIB transition metal dichalcogenides (TMDCs) with generic chemical formula MX 2 (M = Mo, W, etc. and X = S, Se, Te) have been studied as potential candidates for two-dimensional (2D) electronics, spintronics, and valleytronics. Being atomically thin semiconductors, ML-MX 2 is endowed with many fascinating properties, such as intrinsic direct bandgap (E g ~ 1-2 eV) lying within the visible light region, high room temperature carrier mobility (~ 100-700 cm 2 V -1 s -1) and giant spin-orbit coupling (~148-456 meV) close to the K point where the direct bandgap occurs. Moreover, the lattice inversion symmetry is explicitly broken in the monolayers of MX 2, giving rise to a high degree of piezoelectricity (~ 3-7 pm/V). The exciting valley contrasting Berry curvature at the low energy time-reversal valleys at K and -K points in the Brillouin Zone is an exotic phenomenon, allowing to exploit the spin-valley coupled carriers in these multivalley electronic systems. More recently, a new class of monolayer MXY, the so-called Janus derivative of MX 2, has drawn a great deal of research attention, where; X ≠ Y. By breaking the out-of-plane chalcogen sublattice symmetry, novel Rashba-type band splitting and large vertical piezoelectricity has been induced in MXY monolayers. Furthermore, the Rashba spin-orbit interaction is highly strain-tunable in MXY on account of the sensitivity of the dipolar contrast between chalcogen sublattices to the application of strain. The valley contrasting phenomena is also found to be strongly modulated via the application of strain, where the effect is found to be greater for tungsten-based systems. From the family of semiconducting TMDCs, monolayer MoS 2 has drawn a great deal of scientific attention and has been considered to be a perfect semiconducting alternative to semi- metallic graphene. Considering ML-MoS 2 as a candidate system for ab initio studies, the potential of this host semiconductor for electronics, spintronics, and valleytronics has been studied under varying in-plane strain. The elastic strength and mechanical stability under various strain modes have been analyzed in detail. Under the application of uniaxial strain, the conduction band minimum (CBM) of a strained ML-MoS 2 is found to drift nearly 2-times that of the valence band maximum (VBM) about the K-point. The resulting strain induced valley decoherence lifts the valley momentum degeneracy of carriers, thereby affecting the valley contrasting phenomena in a strained MX 2 lattice considerably. The origin of the decoherent valley under applied strain has been ascertained from both geometric and electronic effects, i.e., via alteration in its 2D elasticity and the orbital wave function of low-energy Bloch bands at the respective band-edges. Raman spectroscopy has proven itself to be a non-invasive tool for atomically-thin monolayers under strain. Using first-principles density functional perturbation theory (DFPT), the behavior of crystal phonons in a strained ML-MoS 2 , mainly, the characteristic Raman and IR active vibrations in ML-MoS 2 have been investigated. A large phonon anisotropy and an anomalous frequency shift in the vibrational modes have been observed under the application of strain. 1 The original two-fold frequency degeneracy in its in-plane E 2g Raman active vibration splits 1+ 1− into nondegenerate E 2g & E 2g singlet sub-bands under anisotropic lattice deformation. The vibrational anisotropy is found to scale with the strain-induced elastic anisotropy in its planar stiffness tensors, C 11 and C 22 , and anisotropic phonon electrostatic coupling in a polar semiconductor like ML-MoS 2 . Strong strain-phonon coupling is of crucial importance in accessing the vibrational fingerprints of ML-MoS 2 under the application of various kinds of in- plane strain. The predictive findings presented in this thesis on Group-VIB transition metal dichalcogenides (TMDCs) with a particular focus on ML-MoS 2 and its strain sensitive properties are of paramount interest in future flexible electronics, where the simultaneous occurrence of various quantum DOF in a single integrated electronic system comprising of MX 2 & MXY monolayer crystals can be gainfully exploited.
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