Title:	Energy harvesting in selected semiconducting 2D materials : A theoritical perspective using DFT
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Abstract:	This thesis highlights different kinds of energy conversion in selected atomically thin, two-dimensional (2D) monolayers and their interfaces. Many 2D materials have shown exceptional mechanical, electronic, and catalytic properties. With the advances in their synthesis and device fabrication techniques, low-dimensional materials have been emerging as promising candidates for a variety of applications, such as piezoelectric materials, light-emitting diodes, photocatalysts, solar cells, and thermoelectric materials, etc. In this thesis, monolayers (ML) of Group IVB transition metal dichalcogenides (TMDCs) mainly Mo and W-based dichalcogenides TMDCs, MX2 (M=Mo, W; X= S, Se, Te) have been studied thoroughly for their photocatalytic applications. Also, the charge carrier mobility and the trend in the above monolayers have been properly addressed. Mobility plays an important role in solar energy conversion and nanoelectronics. Despite many astonishing properties, it is still very challenging to find a single 2D having all the desired properties for any device. In order to overcome this challenge, various avenues like the application of mechanical strain or electric field, formation of heterostructures, and Janus structures have been explored. Another class of layered materials known as type II van der Waals (vdW) heterobilayers or heterostructures are formed by stacking different 2D materials using mechanical transfer or chemical vapor deposition techniques. The carrier recombination rate can be significantly lowered in the heterostructures since the electron−hole pairs separate out on the constituent monolayers. Group III-VI-based monolayers and their type II vdW heterobilayers have also been discussed in the thesis where the power conversion efficiency (PCE) and photocatalytic water splitting abilities in these type II vdW heterostructures have been investigated in detail. The power conversion efficiency is found to reach 12.66% and 13.17% in GaTe/InTe and InS/InSe heterostructures, 2 respectively, which are higher than the highest efficiencies reported in organic solar cells (11.7%) and MoS2/p-Si heterojunction solar cells (5.23%). Another group of interesting heterostructures based on M2X; M: Na/Cs/K, X: O/S/Se/Te materials have also been explore for solar cell applications where K2O/Cs2O, K2S/Cs2S and K2Se/Cs2S structures exhibit a high-power conversion efficiency of 21.56%, 19.31% and 16.43% respectively along with a high carrier mobility > 103 cm2/V.s. Recently, a new member in the family of 2D materials, namely, the Janus structures, has been introduced and has become a hot topic among researchers. In 2017, Lu et al successfully synthesized MoSSe by controlled sulfurization of the top layer of MoS2 by Se but the theoretical prediction for the existence of such materials was given four years back in 2013 by Cheng et al. We have systematically studied 1H and 1T based 2D Janus transition metal dichalcogenides (MXY; M: Mo/W/Hf/Zr, X/Y: S, Se, Te) and also their photocatalytic abilities and potential for solar cell applications. The stability of such heterobilayers has been confirmed by various mechanical, energetical, and dynamical aspects. Hence the theoretical study suggests the feasibility for the fabrication of such monolayers and heterobilayers. In addition to photocatalysis and solar cell applications, in the quest to find better 2D piezoelectric materials, we have theoretically designed a novel 2D material ScAgP2S6 which is mechanically, thermodynamically, and lattice dynamically stable. The application of 2D materials in thermoelectric devices has also been studied. The thermoelectric properties of the HfN2 monolayer have been evaluated by using the semi-classical Boltzmann transport theory of electrons and phonons. It exhibits low lattice thermal conductivity of 0.49 □□−1□−1 at room temperature and excellent waste heat to electricity conversion efficiency (Figure of merit, ZT= 2.28). Moreover, HfN2/MoTe2 van der Waals heterostructure (vdWH) based excitonic solar cell has been designed, which is found to be stable. It shows a direct semiconducting bandgap with a type-II band 3 alignment. The very high-power conversion efficiency of 21.44 % is achieved for the HfN2/MoTe2 van der Waals heterostructure.
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