Title:	FIRST-PRINCIPLES QUANTUM MECHNICAL INSIGHTS INTO EMERGING 2D MATERIALS FOR FUTURISTIC ELECTRONICS AND ENERGY
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Abstract:	This thesis encompasses a broad range of cutting-edge research areas extending from energy harvesting from renewable resources to futuristic electronic devices utilizing novel properties and different degrees of freedom of electrons which emerge in atomically thin two-dimensional (2D) semiconductors and their van der Waals heterostructures. Specifically, nanoelectromechanical energy conversion (piezoelectric effect), solar energy harvesting (photovoltaic effect) as well as spintronics and valleytronics based on 2D monolayers have been presented in the thesis. Atomic-scale insights into the electronic, optical, mechanical, piezoelectric, spintronic and valleytronic properties in selected 2D materials have been obtained through the lens of first-principles state-of-art density functional theory (DFT) based approaches. The significance of integrating their different properties in designing a multifunctional device for advanced applications has also been emphasized. The thesis is organized in the following way. The first part of the thesis is concentrated on energy harvesting, particularly, on the generation of electricity from mechanical energy as well as spintronics device applications emanating from the Rashba effect. The simultaneous occurrence of gigantic piezoelectricity and Rashba effect in two-dimensional materials are unusually scarce. Inversion symmetry occurring in MX 3 (M= Ti, Zr, Hf; X= S, Se) monolayers is broken upon constructing their Janus monolayer structures MX 2 Y (X≠Y=S, Se), thereby inducing a large out-of-plane piezoelectric constant, d 33 (~68 pm/V) in them. d 33 can be further enhanced to a super high value of ~1000 pm/V upon applying vertical compressive strain in the van der Waals bilayers constituted by interfacing these Janus monolayers [1]. The 2D Janus transition metal trichalcogenide monolayers and their bilayers presented herewith in this Ph.D. work, straddle giant Rashba spin splitting and ultrahigh piezoelectricity, thereby making them immensely promising candidates in the next generation electronics, piezotronics and spintronics devices. A detailed theoretical investigation has been conducted for a quantitative study and in-depth understanding of the desired parameters. Next, h-MN (M=Nb, Ta) monolayers have been investigated which are found to host valley physics together with Rashba effect due to the presence of strong spin-orbit coupling and absence of inversion symmetry [2]. The search for new two-dimensional (2D) semiconductors with strong spin-orbit coupling, merging Rashba effect with valley physics, is essential for advancing the emerging fields of spintronics and valleytronics. Other than chargeand spin degrees of freedom (DOF), valley DOF (+K, -K) of electron can be used for information storage in the domain of valleytronics. h-NbN (TaN) monolayers which exhibit a strong spin-orbit coupling leading to a large valley spin splitting (VSS) ~112 (406) meV at its conduction band edge has been investigated for its application in valleytronics. Valleytronic and spintronic properties in the studied monolayers are found to be superior to that in h-MoS 2 and Janus MoSSe monolayers and are therefore proposed for an effective coupling of spin and valley physics. The final part of the thesis is focussed on energy harvesting, particularly, on the generation of electricity from solar radiation using two-dimensional vdW hetero-bilayers of ZrS 3 /MS 2 and ZrS 3 /MXY (M=Mo, W; X, Y=S, Se, Te; X ≠ Y) [3]. Electronic, optical, and transport properties in these 2D vdW hetero-bilayers have been investigated in-depth for the purpose of exploring their prospects for applications in photovoltaics. The comprehensive study presented in this Ph.D. work illustrates a new avenue for an efficient solar energy conversion at the nanoscale based on ZrS 3 /MS 2 and ZrS 3 /MXY vdW hetero-bilayers in ultrathin, 2D excitonic solar cells. The thesis emphasises the fundamental and technological significance of sustainable and alternative energy harvesting as well as next-generation electronic devices through efficient use and engineering of 2D materials. The approach implemented in the Ph.D. work involves in studying the several entangled properties in a multifunctional material, thereby enabling to draw a systematic correlation between them
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