Title:	ATOMIC-SCALE INSIGHTS INTO ENERGY CONVERSION IN TWO- DIMENSIONAL TRANSITION METAL DICHALCOGENIDE MONOLAYERS FROM AB-INITIO STUDIES
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Abstract:	This thesis highlights different kinds of energy conversion in atomically thin, two-dimensional (2D) transition metal dichalcogenide (TMDC) monolayers. More precisely, nanoelectromechanical energy conversion (piezoelectricity), scavenging waste heat into electricity (thermoelectricity) and solar energy harvesting (artificial photosynthesis) based on 1T-MX 2 (M=Zr, Hf; X = S, Se, Te) and 1H-MoS 2 monolayers have been addressed in the thesis. As carrier mobility commonly influences all these kinds of energy conversion, it has also been thoroughly investigated as well. Atomic-scale understanding reached via state-of-art first-principles calculations based on density functional theory (DFT) has been employed to uncover their electronic, optical, mechanical, piezoelectric and thermoelectric properties. First of all, the thesis introduces the occurrence of piezoelectricity in 2D semiconducting transition metal dichalcogenide monolayers, such as 1H-MoS 2 , which arises from the breaking of inversion symmetry. However, pristine, semiconducting 1T-MX 2 (M=Zr, Hf; X = S, Se, Te) monolayers are intrinsically centrosymmetric and hence, non-piezoelectric. This inversion symmetry is broken in their Janus monolayer (non-centrosymmetric) structures, leading to the emergence of a high level of piezoelectricity in them. It brings along a new dimension in nanoscale piezoelectricity, as the origin of this piezoelectricity is predominantly ionic in nature, in contrast to 1H-MoS 2 monolayer, where it is of electronic character. Next, the mechanism underlying the compressive strain induced enhancement in thermoelectric power-factor has been unveiled in single-layer MoS 2 , using density functional theory coupled to Boltzmann transport equation. A synergic coupling between the lattice vibrational properties and high Born effective charges in monolayer Hafnium dichalcogenides, such as HfS 2 , HfSe 2 and their Janus derivative HfSSe, have been explored to reach the origin of ultralow lattice thermal conductivity in them. Finally, the effect of strain and pH on the artificial photosynthetic properties in single layer MoS 2 has been comprehensively studied in terms of band edges straddling the water redox potential, CO 2 reduction levels, optical conductivity, absorbance, carrier mobility and carrier mobility ratio in order to ascertain the type and magnitude of strain under which photocatalytic activities are optimally enhanced. The thesis stresses the importance of finding sustainable, clean and alternative energies through efficient use and engineering of 2D materials. The approach adopted in the Ph.D. work consists in studying the several intertwined properties in a multifunctional material, thereby enabling to draw a systematic correlation between them.
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