

Tribo-piezoelectric Nanogenerators for Energy Harvesting: a first principles study

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ABSTRACT

Two-dimensional transition metal dichalcogenides (TMDs) are highly promising candidates for various applications due to their unique electrical, optical, mechanical, and chemical properties. Furthermore, heterostructures consisting of TMDs with metals, oxides, and conductive materials have attracted significant research interest due to their exceptional electronic properties. In this study, we utilized density functional theory to investigate those electronic and transport properties, which are relevant for the application of tribo piezoelectricity in creating novel nanogenerators: an interdisciplinary approach with promising implications. The results of the study demonstrate that the enhancement of charge transfer between layers and the orbital contribution to the Fermi level under applied strain in MoS/IrO, MoS/TiO, MoS/WTe, and MoTe/WS heterostructures is noteworthy. Additionally, non equilibrium Green's function calculations of electron transport properties provide valuable insights into the behaviour of these materials under different conditions. While MoS/IrO and MoS/TiO hetero-bilayers are unsuitable due to their tendency to exhibit large current flow with increasing voltage, others like MoS/WTe and MoTe/WS hetero bilayers show promise due to their ability to prevent voltage drop. The presented innovative concept of utilizing compressive strain of TMD bilayers to generate a tribo-piezoelectric effect for nanogenerators has a potential to contribute to the development of efficient and sustainable energy harvesting devices.