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MoTe₂ growth by Tellurization and its Tunable Band Alignment of MoTe₂ with SiO₂ interface using internal photoemission spectroscopy

J. Chemical functionalization of 2D materials

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Abstract

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Two-dimensional transition metal ditellurides (2D-TMTs) exhibit unique characteristics promising device applications in various technological fields, spanning from opto- and nano-electronics to memories[1] Among many 2D-TMTs, molybdenum ditelluride (MoTe₂) attracts particular attention due to its polymorphic character resulting in semiconducting 2H (trigonal prismatic coordination) and metallic 1T' (distorted octahedral coordination) phases which is subjected to structural distortion to the Td phase (orthorhombic). [1-3] MoTe₂ exhibits a stable biphasic character in artificially synthesizable 2H and 1T' polytypes inherently distinguished in their electronic band structure (semiconducting and metallic, respectively). Phase-engineered transition metal transition (TMT) materials that incorporate van der Waals interactions and intrinsically absent dangling bonds demonstrate the potential to design electronic and optoelectronic devices with exceptional performance.[4] However, it is not clear how they electronically interfaced with the technology relevant substrate like SiO₂ or with another TMT phase, and what impact it has on an electronic device layout. Therefore, it is critically

important to characterize the band alignment of these Van der Waals heterojunction that enables to control the electronic transport in the heterostructures. [4] In this work, we demonstrate large scale and accurate phase-controlled synthesis of 1T' and 2H MoTe₂ films with its correlation between the concentration gradient of Te vapor and the deposited MoTe₂ morphology and coverage. [2] Next, we investigate the tunable energy band alignments of the phase-engineered 1T', 2H and vertical hybrid 1T'/2H few layered MoTe₂ measured by internal photoemission spectroscopy (IPE) which allows one to determine the energy barrier height between the valence band (VB) top edge of MoTe₂ and the SiO₂ conduction band (CB) bottom. This experiment reveals the band gap opening in 2H, 1T' and hybrid 1T'/2H-MoTe₂ and provides an estimate of the barrier height for holes at the polytypic 1T'/2H-MoTe₂ interface. Notably, transition to 2H-MoTe₂ is accompanied by a considerable energy shift of the VB top edge of approximately 0.4 eV as compared to 1T'-MoTe₂, indicating the opening of a band gap. This work offers a vital insight that can be optimized depending on the target device and opens a window for the MoTe₂ few layered materials as a building block for high-performance electronic and memory applications.

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References

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