Band Structure Modulation of Monolayer TMDs using Pressure

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Semiconducting transition metal dichalcogenides (TMDs), a group of two-dimensional (2D) materials, are promising candidates for next-generation optoelectronics and energy harvesting devices.[1-3] However, effective band offset engineering is required to implement practical structures with desirable functionalities. Here, we explore the pressure-induced modulation of band structure and explore the possibility of band alignment engineering through different composition in monolayer WS_2 and $Mo_{0.5}W_{0.5}S_2$. Hydrostatic compressive strain is applied in a diamond anvil cell (DAC) apparatus, and combined with theoretical calculation to understand the band edge evolution. Compared with previously reported MoS_2,[4] higher W composition in $Mo_{(1-x)}W_{(x)}S_2$ contributes to a greater pressure-sensitivity of direct band gap opening, with a maximum value of 54 meV/GPa in WS_2. Interestingly, while the conduction band minima (CBMs) remains largely unchanged after the rapid gap increase, valence band maxima (VBMs) significantly rise above the initial values. It is suggested that the pressure- and composition-engineering could introduce a wide variety of band alignments, and allow to construct precise structures with desirable functionalities. No structural transition is observed during the pressure experiments, implying the pressure could provide arbitrary modulation of band offset.

References:

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