$PbI_2/MoSe_2$  van der Waals heterostructures: Engineering heterointerface and optoelectronics

Two-dimensional (2D) semiconducting materials have attracted significant attention due to their exotic electronic and optoelectronic properties dependent on the structures. Furthermore, 2D semiconductors comprising vertically stacked heterostructure show substantial potential for bandgap engineering by controlling the van der Waals interactions of the given layer configurations, which is impossible in conventional 3D crystalline semiconductors. Herein, we demonstrate the heterostructures composed of 2D MoSe<sub>2</sub> and PbI<sub>2</sub>, with distinct interface configurations. First, nanostructures composed of PbI<sub>2</sub> multilayers were prepared by VLS growth, which showed two different stacking orientations(i.e., [0001] and [-12-10]). They were transferred onto the CVD grown MoSe<sub>2</sub> monolayers, resulting in the distinct heterointerface. We confirmed that PL is dependent on the interface configurations between MoSe<sub>2</sub> and PbI<sub>2</sub>. An ab initio calculation further supported that the band alignments are contingent upon the atomic arrangement at the heterointerface. Our results contribute to the development of the bandgap-engineered vdW heterostructures.