

Electronic Supplementary Information

Enhanced carrier separation in ferroelectric In₂Se₃/MoS₂ van der Waals heterostructure

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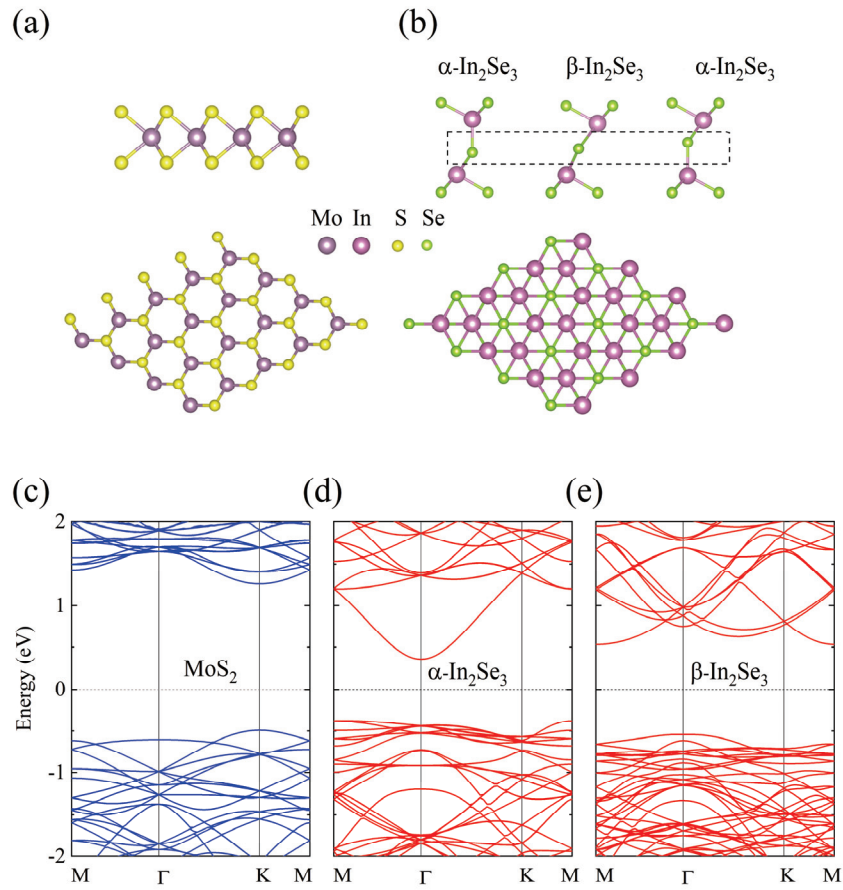


Fig. S1 Top and side views of (a) MoS₂ and (b) α-In₂Se₃(β-In₂Se₃) monolayers. The band structures of monolayer (c) MoS₂, (d) α-In₂Se₃ and (e) β-In₂Se₃.

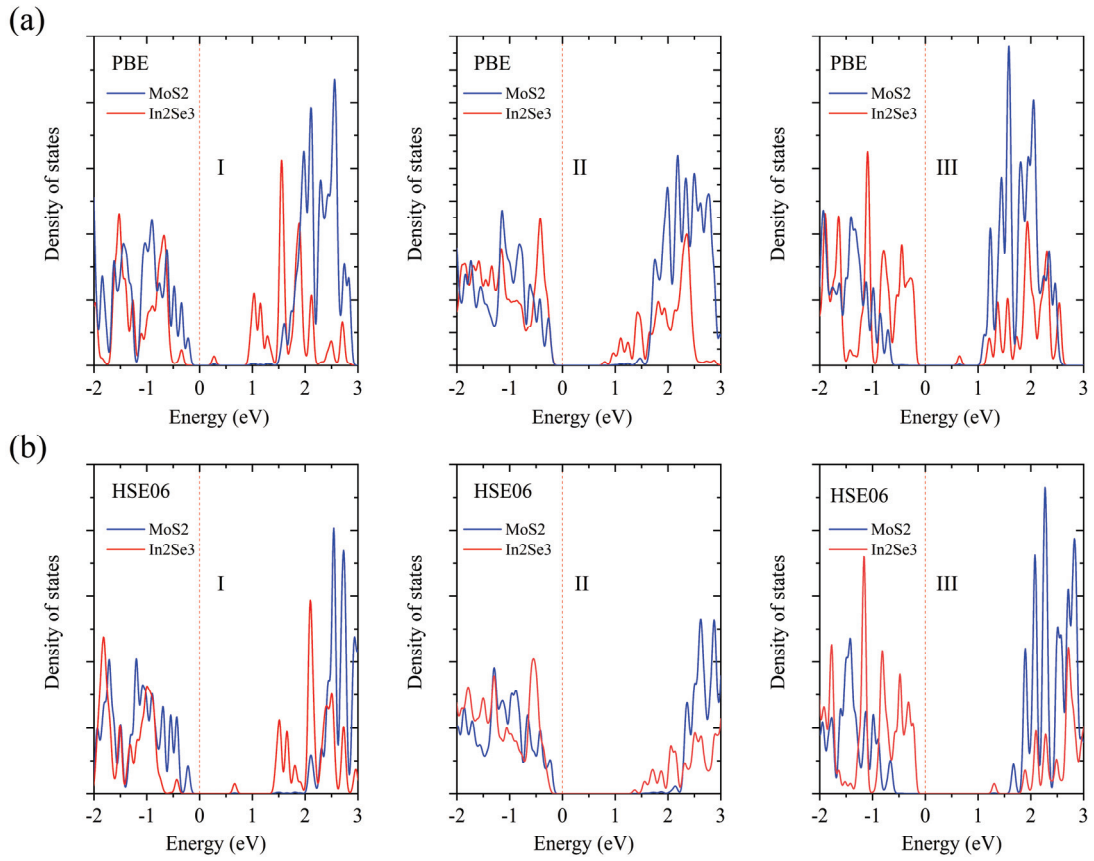


Fig. S2 Calculated PDOS of the In₂Se₃/MoS₂ (I, II, III) heterostructures based on PBE (a) and HSE06 (b).

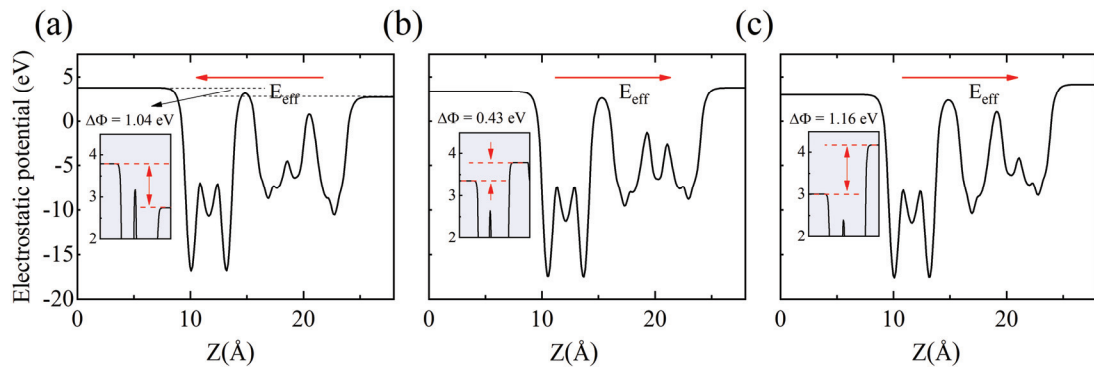


Fig. S3 Surface potential differences for (a) In₂Se₃/MoS₂ (I), (b) In₂Se₃/MoS₂ (II) and (c) In₂Se₃/MoS₂ (III). The E_{net} represent the effective electric field across the heterostructure interface.

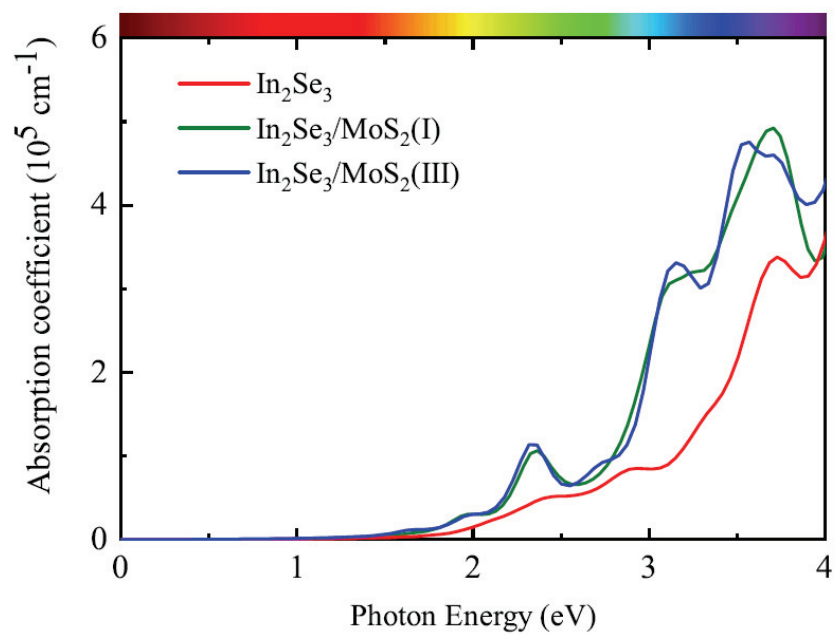


Fig. S4 The optical absorption of the $\text{In}_2\text{Se}_3/\text{MoS}_2$ (I, III) heterostructures and the isolated In_2Se_3 monolayer, based on HSE06 calculations.