Supplementary material

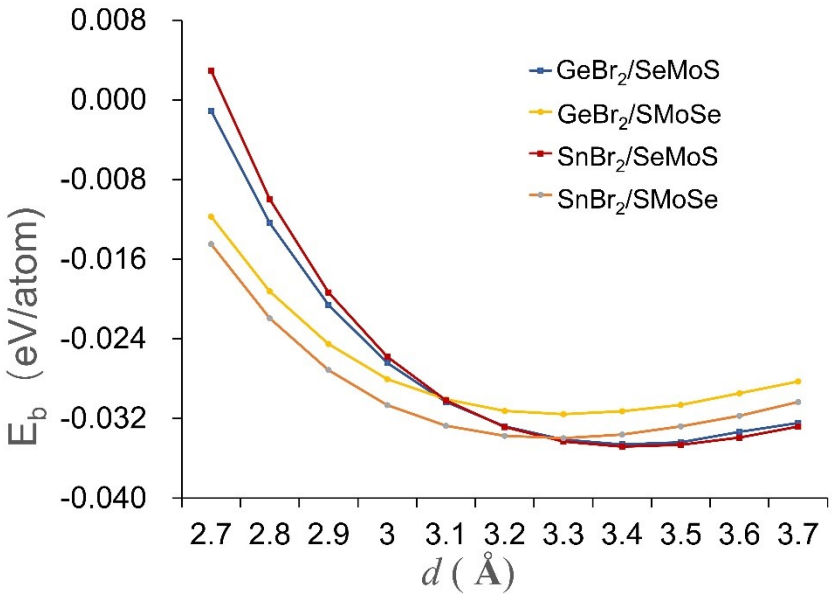

Fig. S1. Binding energy (E_b) as a function of interlayer distance d for $CsXBr_3$ /Janus MoSSe heterostructures.

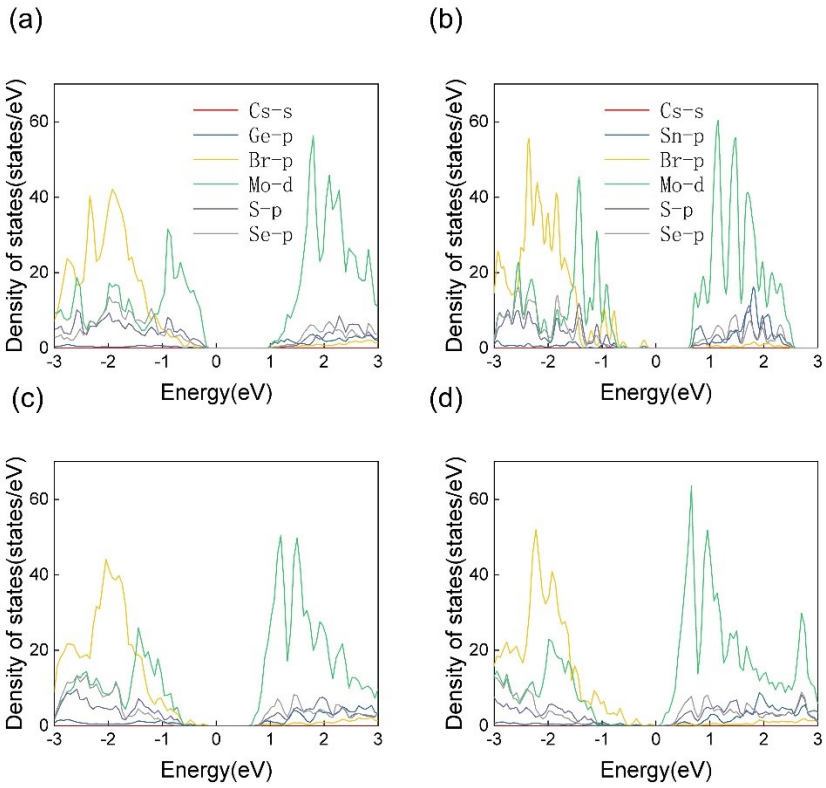

Fig. S2. Projected density of states (PDOS) of (a) $GeBr_2$/SeMoS, (b) $SnBr_2$/SeMoS, (c) $GeBr_2$/SMoSe, and (d) $SnBr_2$/SMoSe heterostructures.

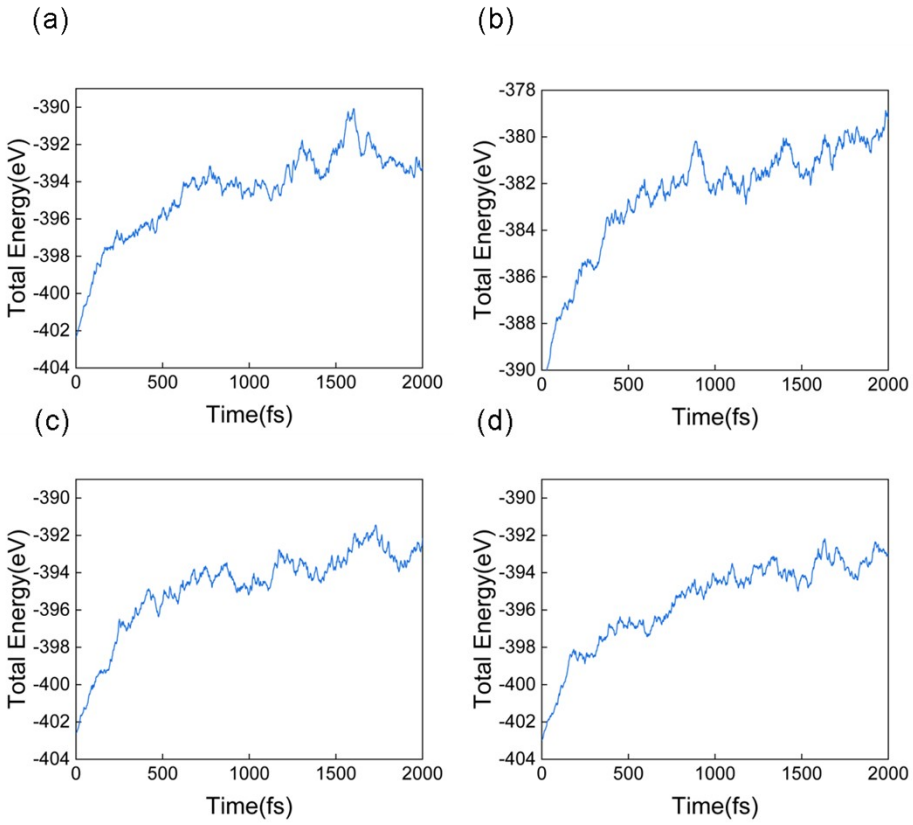

Fig. S3. Ab initio molecular dynamics (AIMD) of (a) $GeBr_2$/SeMoS, (b) $SnBr_2$/SeMoS, (c) $GeBr_2$/SMoSe, and (d) $SnBr_2$/SMoSe heterostructures.

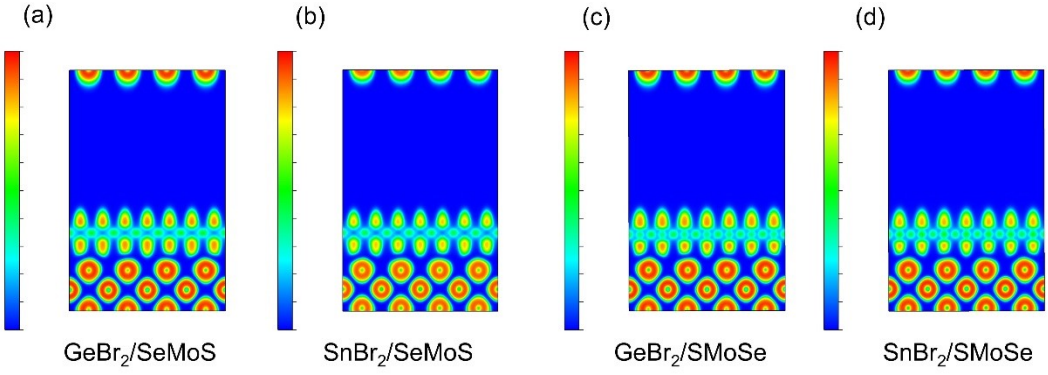

Fig.S4. The electron localization function (ELF) of (a) $GeBr_2$/SeMoS, (b) $SnBr_2$/SeMoS, (c) $GeBr_2$/SMoSe, and (d) $SnBr_2$/SMoSe heterostructures.