Supporting Information (SI) for

# Electronic Properties and Interfacial Engineering of metal-semiconductor 1T-, 2H - $Ta_2B$ MBene/Janus MoSSe Heterostructures

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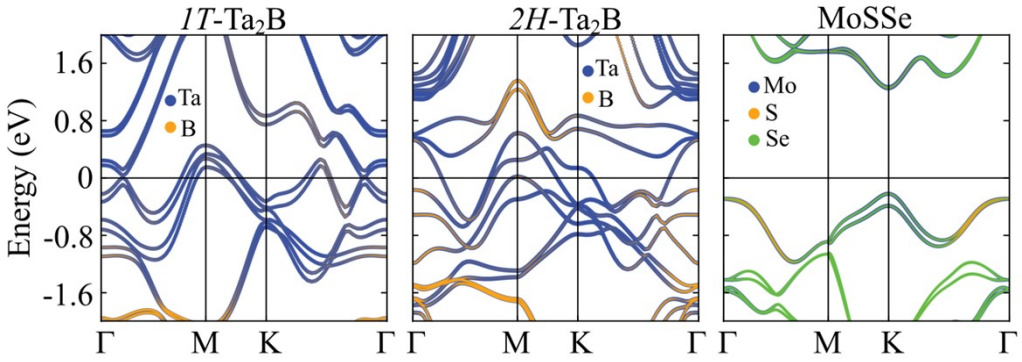


Figure S1. Projected band structures of 1T-$Ta_2B$, 2H-$Ta_2B$ and Janus MoSSe monolayers given by PBE+SOC calculations.

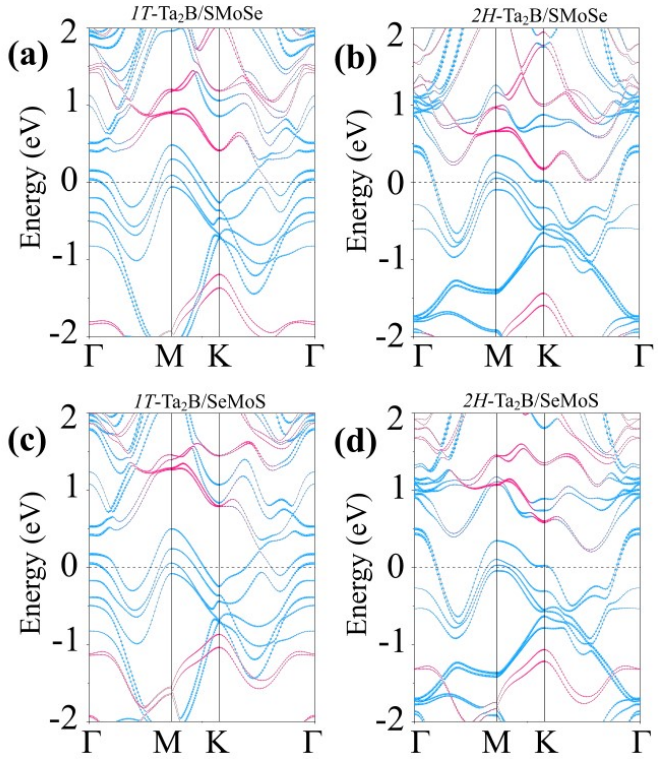


Fig. S2. PBE+SOC projected band structure of $Ta_2B$/SMoSe for (a) 1T-AB1 and (b) 2H-AB1 and $Ta_2B$/SeMoS for (c) 1T-AB1 and (d) 2H-AB1 stacking configurations

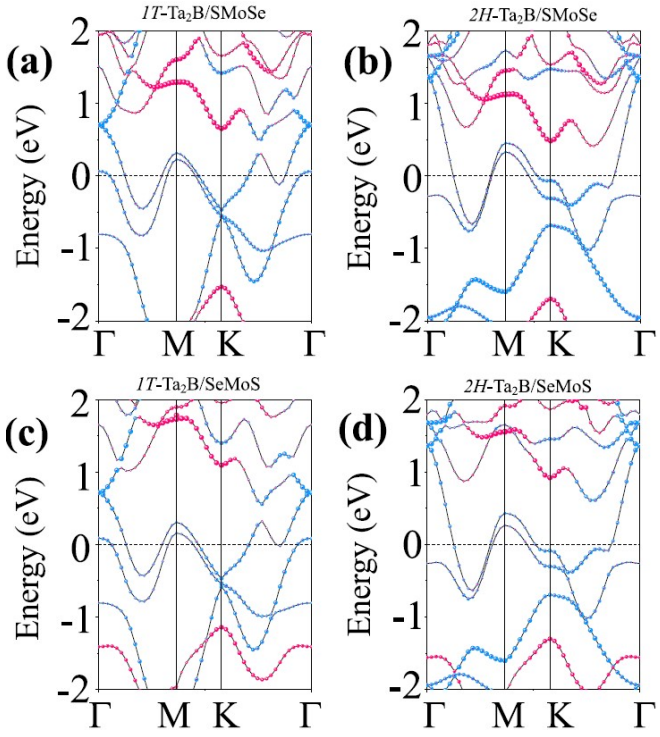


Fig. S3. HSE06 projected band structure of $Ta_2B$/SMoSe for (a) 1T-AB1 and (b) 2H-AB1 and $Ta_2B$/SeMoS for (c) 1T-AB1 and (d) 2H-AB1 stacking configurations

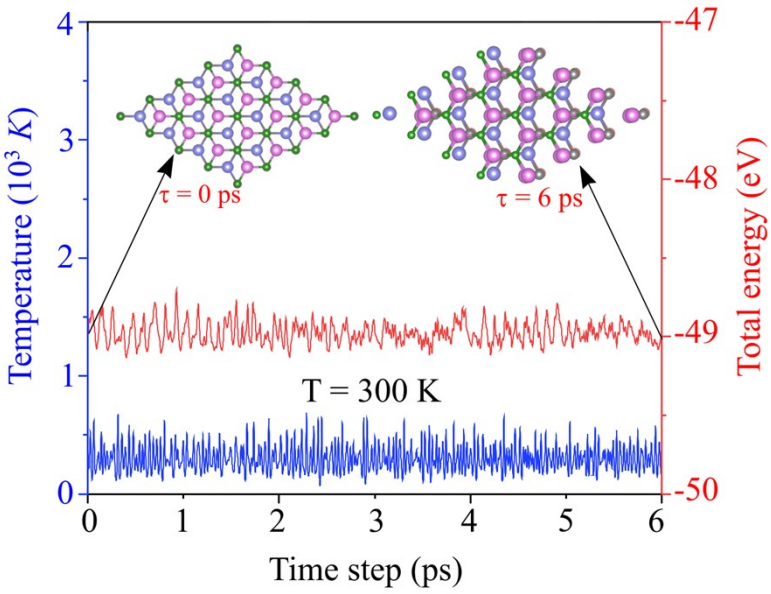


Fig. S4. The fluctuations in temperature and total energy of 2*H*-$Ta_2B$/SeMoS heterostructure for the most energetically favorable 2H-AB1 stacking arrangement.