Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supporting Information (SI)

Theoretical prediction of electronic properties and contact barriers in metal/semiconductor NbS_2/Janus MoSSe van der Waals heterostructure

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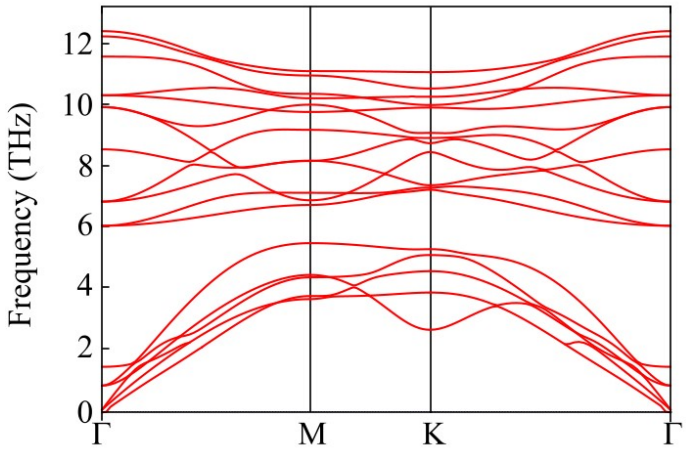

Fig. S1. Phonon dispersion curves of NbS_2/MoSSe heterostructure for the most energetically favorable stacking configuration.

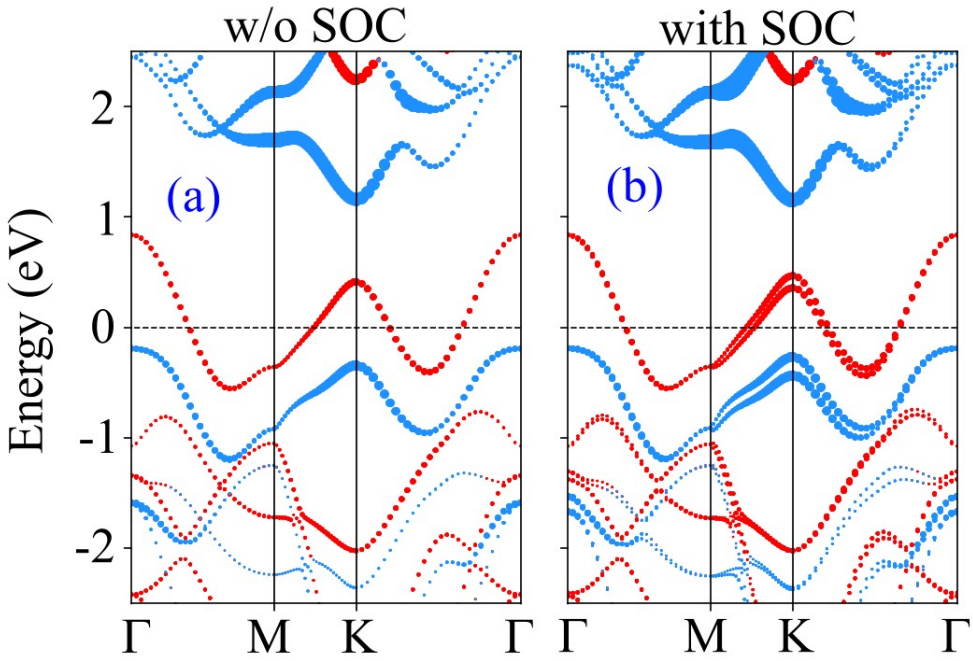

Fig. S2. Projected band structures of NbS_2/MoSSe heterostructure for the most energetically favorable stacking configuration (a) without (w/o) SOC and (b) with SOC effect.

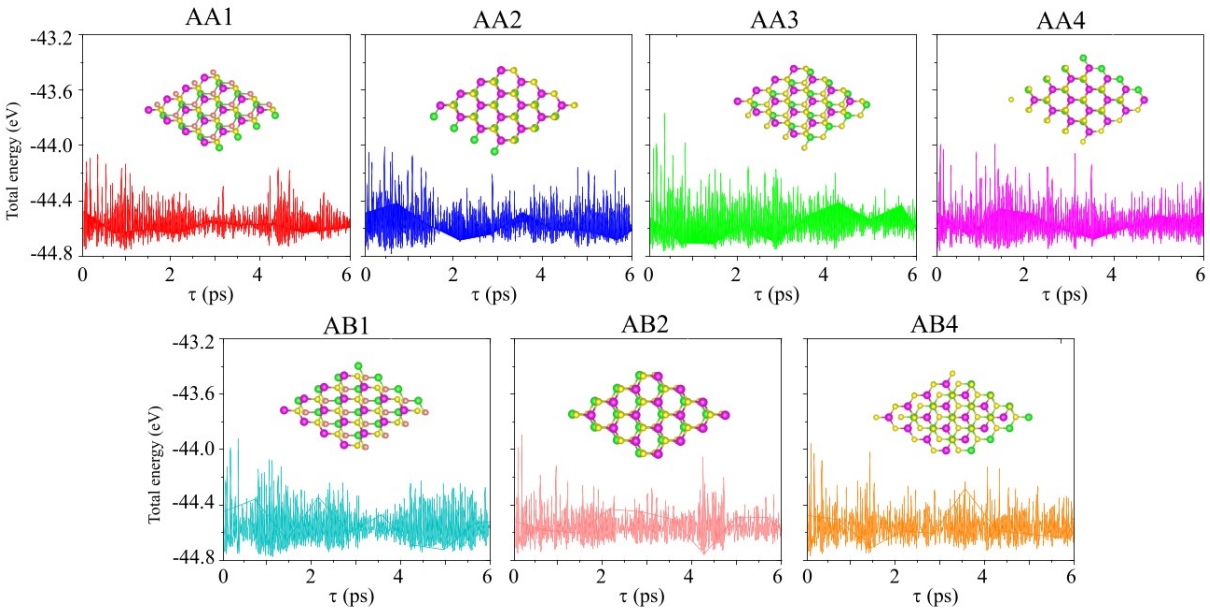

Fig. S3. The fluctuation in total energy as a function of time steps of the NbS_2/MoSSe heterostructure for different stacking configurations. The insets represent the atomic structure of heterostructure after heating to 6 ps.