Electronic supplementary information (ESI)

Impact of edge on interfacial interactions and efficient visible-light photocatalytic activity of metal-semiconductor hybrid 2D materials

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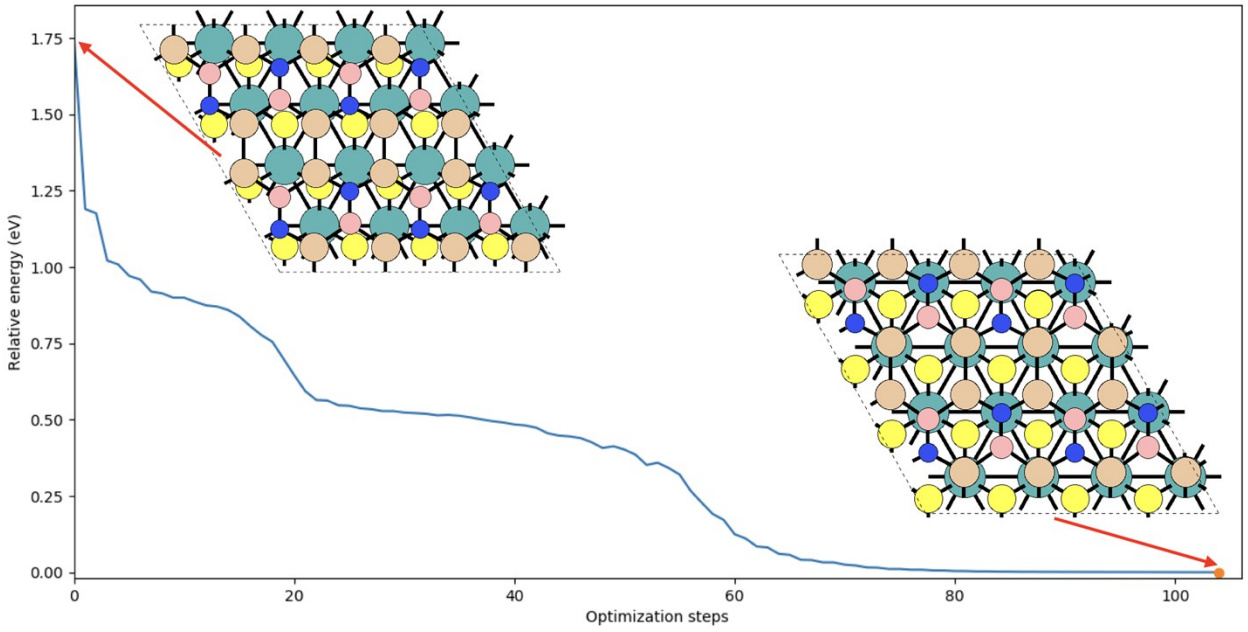

Figure S1. The relative energy profile of mSi_2BN/MoS_2 heterostructure under vdW interactions between Si_2BN and MoS_2 monolayer.

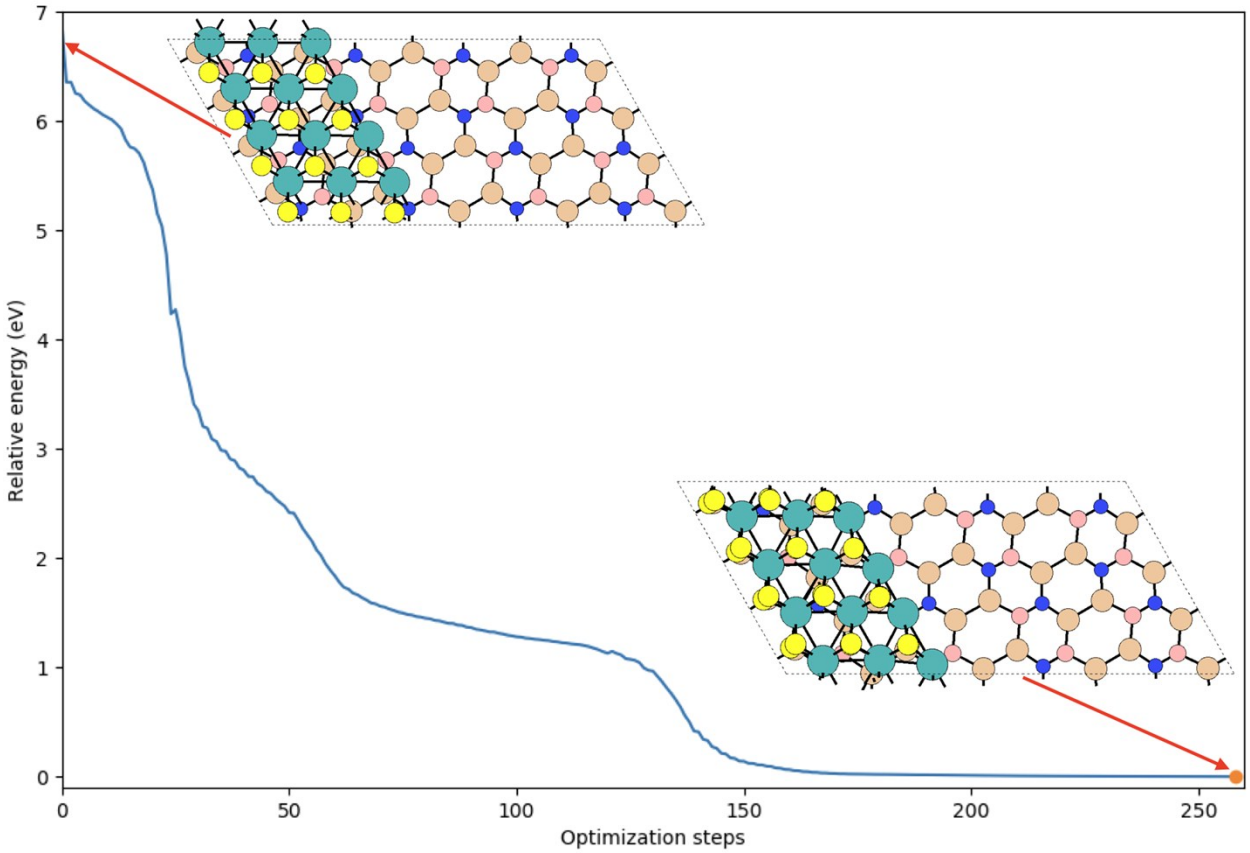

Figure S2. The relative energy profile of rSi_2BN/MoS_2 heterostructure under vdW interactions between Si_2BN monolayer and MoS_2 nanoribbon.

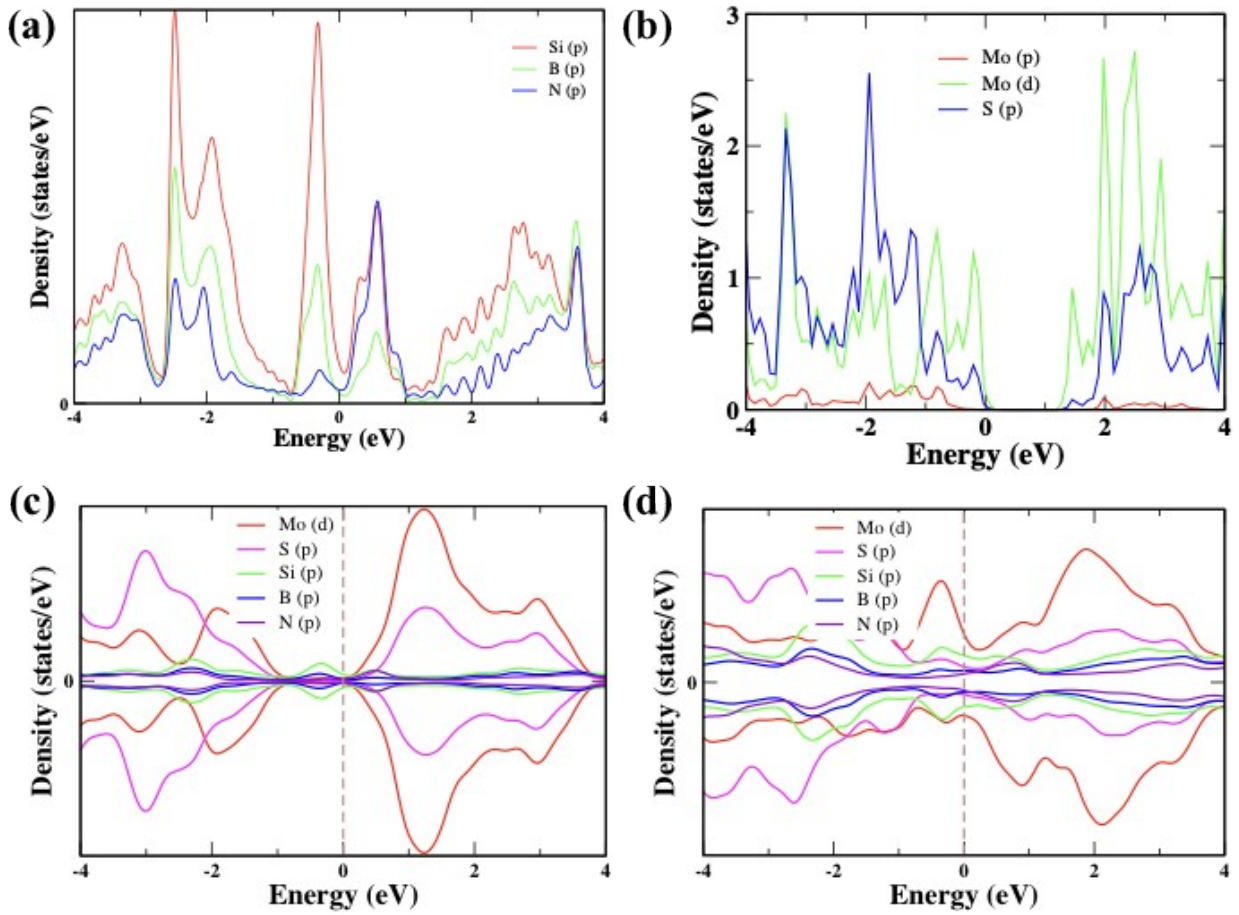

Figure S3. The projected density of states of pristine (a) Si_2BN monolayer, (b) MoS_2 monolayer. The orbital-decomposed density of states of heterostructure of (c) mSi_2BN/MoS_2 and (d) rSi_2BN/MoS_2 system. The Fermi energy is set at zero.

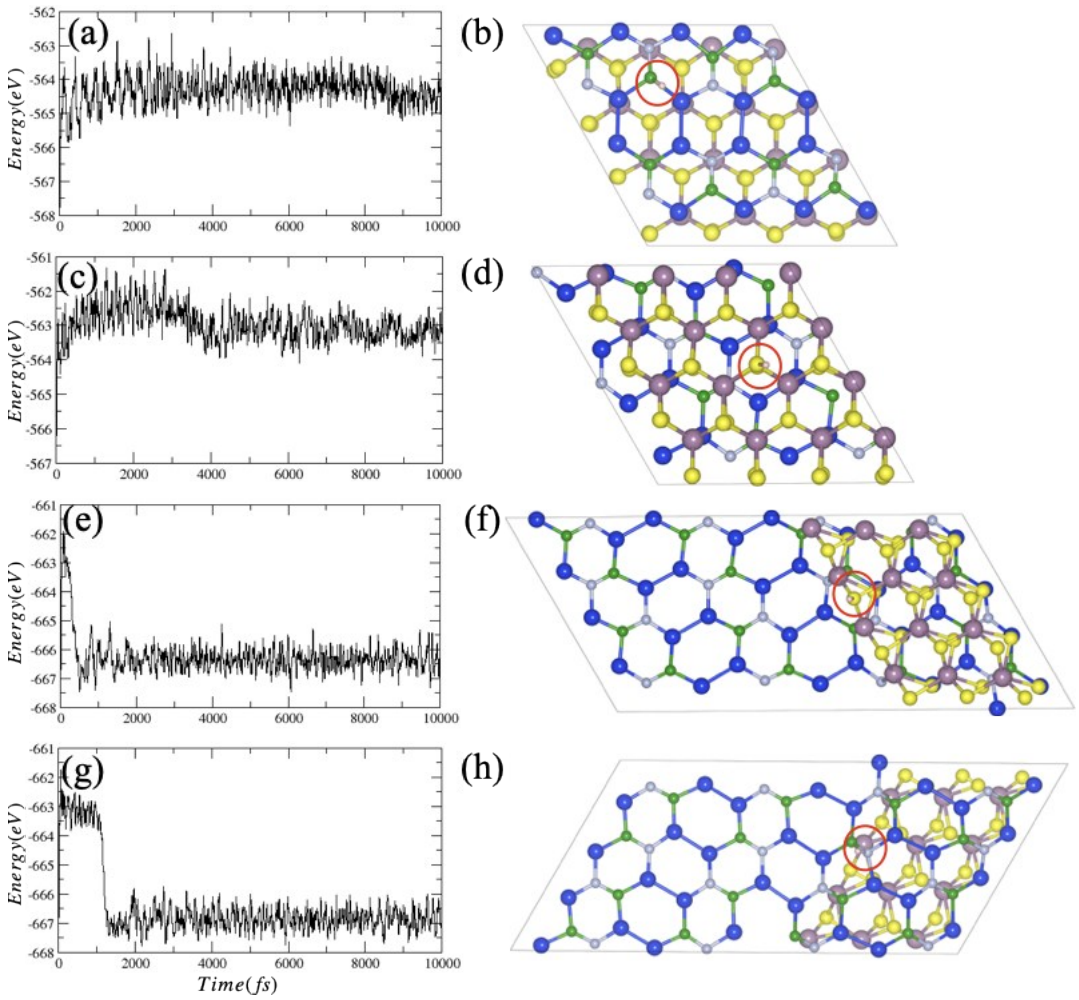

Figure S4. The change of total energy at 300 K as a function of time for the considered sheet. The inserts present the relaxed MoS_2/Si_2BN monolayer and ribbon after the different dynamic simulations, along with their structure distortion. (a) Total energy variation of MoS_2/Si_2BN monolayer and H atom absorbed on Si_2BN side and (b) corresponding optimized structure in which H atom presented at the same position like Figure 6 (see in the main manuscript). (c) Total energy variation of MoS_2/Si_2BN monolayer and H atom absorbed on MoS_2 side and (d) corresponding optimized structure, (e) total energy variation of MoS_2/Si_2BN ribbon and H atom absorbed on MoS_2 side and (f) corresponding optimized structure, (g) total energy variation of MoS_2/Si_2BN ribbon and H atom absorbed on Si_2BN side and (h) corresponding optimized structure in which H atom presented at the same position like Figure 6 (see in the main manuscript).

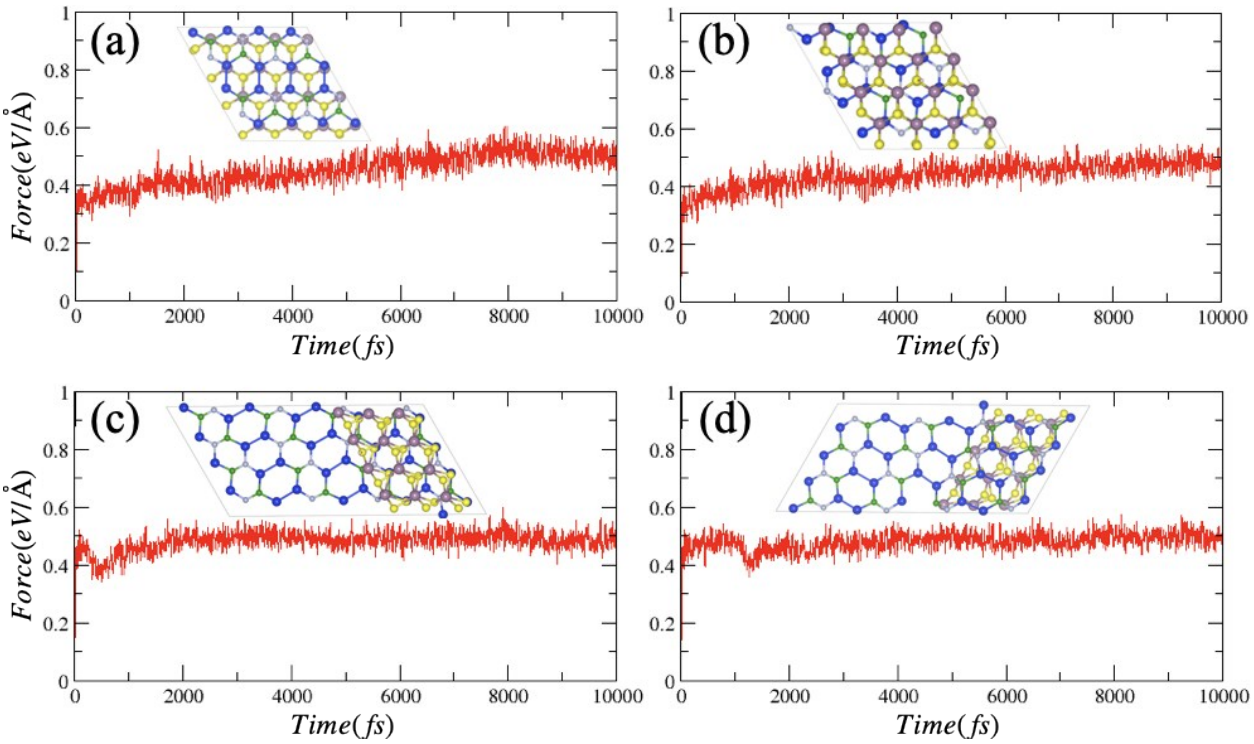

Figure S5. The fluctuation of average force at 300 K as a function of time for the considered sheet. The inserts present the relaxed MoS_2/Si_2BN monolayer and ribbon after the different dynamic simulations, along with their structure distortion. (a) Average force variation of MoS_2/Si_2BN monolayer and H atom absorbed on Si_2BN side, (b) average force variation of MoS_2/Si_2BN monolayer and H atom absorbed on MoS_2 side (c) average force variation of MoS_2/Si_2BN ribbon and H atom absorbed on MoS_2 side (d) average force variation of MoS_2/Si_2BN ribbon and H atom absorbed on Si_2BN side in which H atom presented at the same position like Figure 6 (see in the main manuscript).