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Supplementary Materials

Manipulable Electronic and Optical Properties of Two-Dimensional $MoSTe/MoGe_2N_4$ van der Waals Heterostructures

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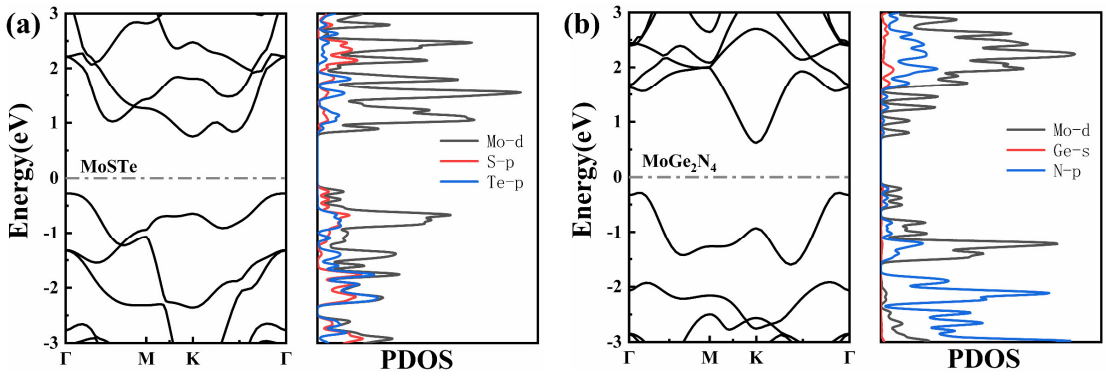


Figure S1. Band structures and PDOS of (**a**) Janus MoSTe monolayer and (**b**) $MoGe_2N_4$ monolayer, respectively. The Fermi levels are set to zero.

Table S1. : Binding energies (E_b) of the optimized $MoSTe/MoGe_2N_4$ vdWH for the twelve different stacking patterns.

Heterostructure	Te_1	Te_2	Te_3	Te_4	Te_5	Te_6
E_b (meV)	-6.7680	-6.7679	-6.7671	-6.7710	-6.7670	-6.7708

Heterostructure	S_1	S_2	S_3	S_4	S_5	S_6
E_b (meV)	-6.7396	-6.7407	-6.7405	-6.7434	-6.7427	-6.7394

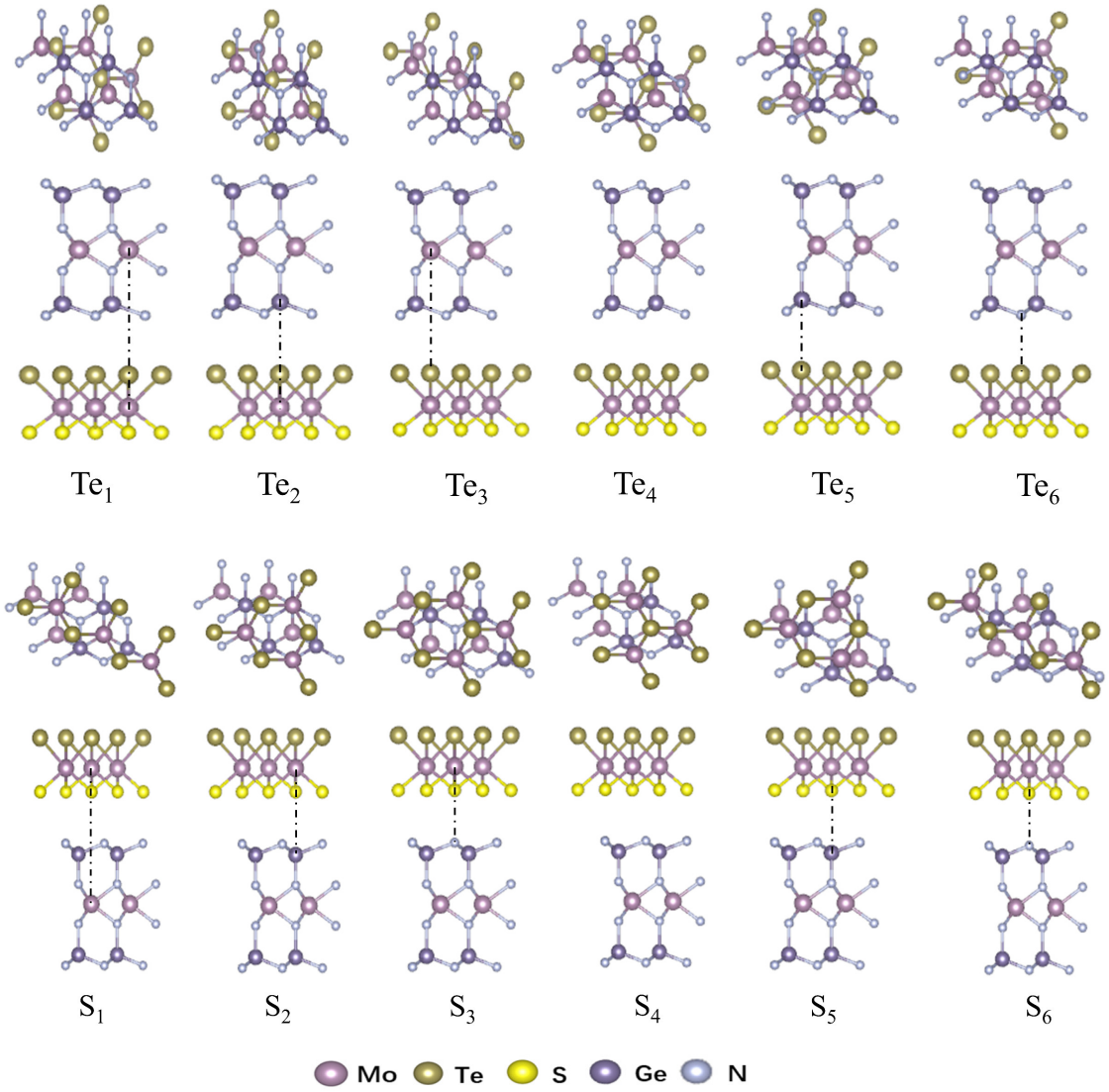
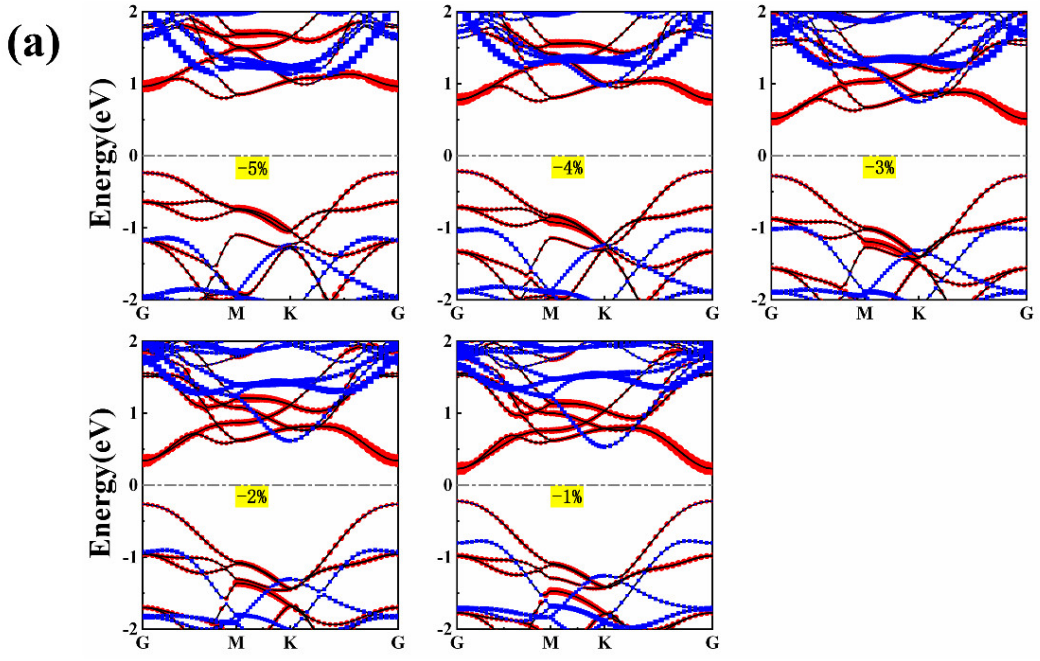
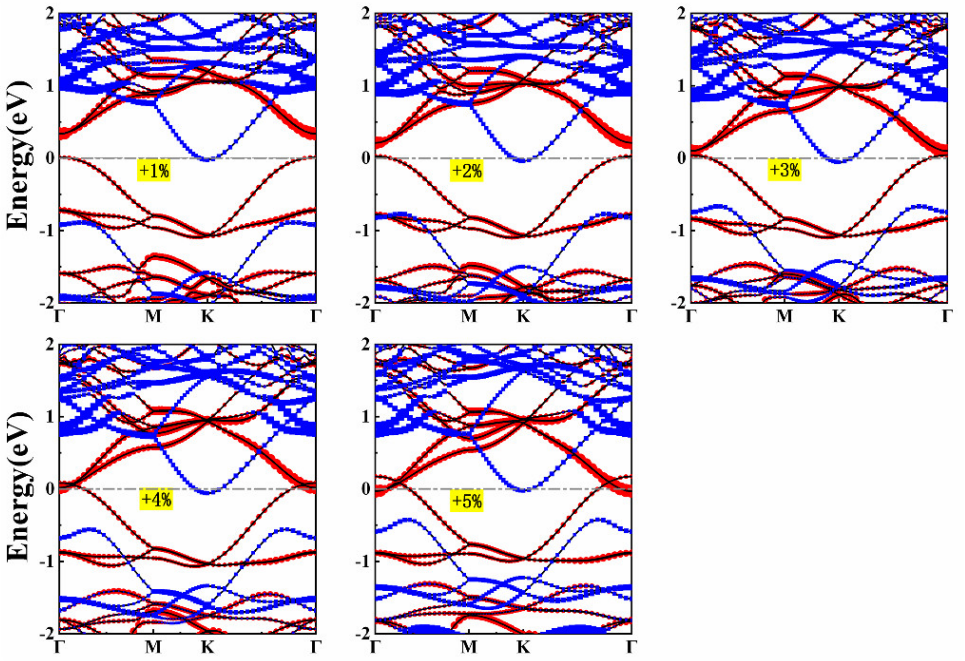


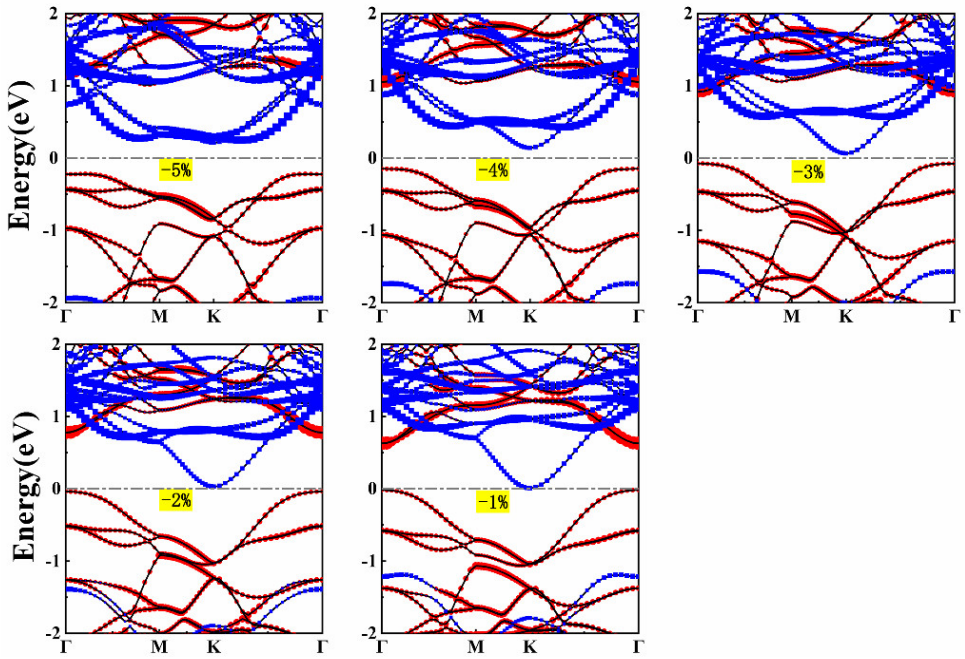
Figure S2. The optimized top and side views of the MoSTe/$MoGe_2N_4$ vdWH for twelve different stacking patterns.



(b)



(c)



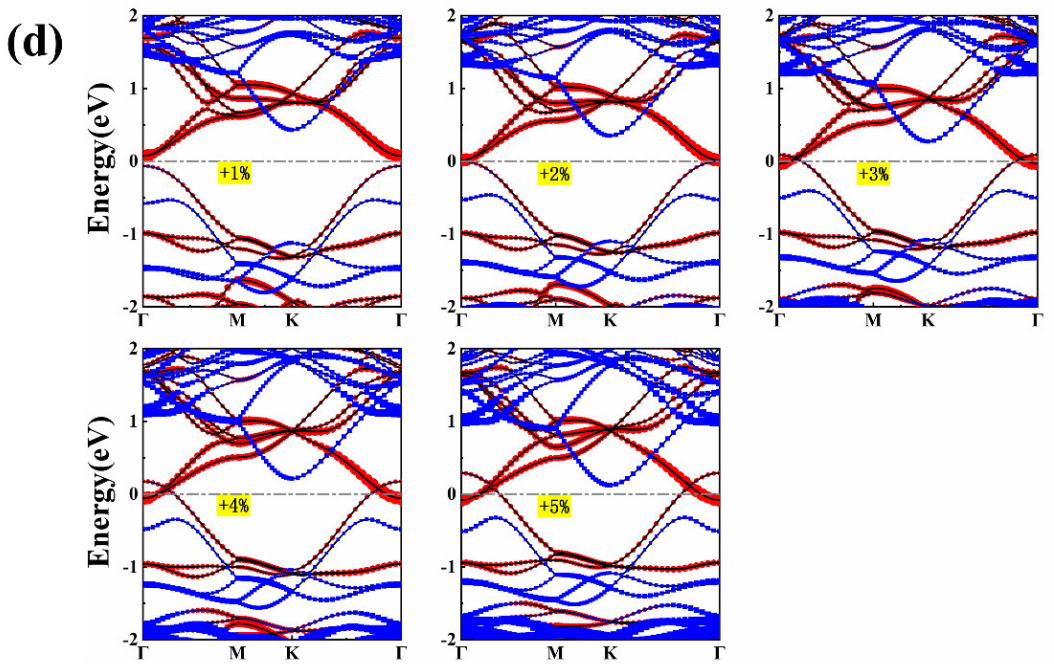
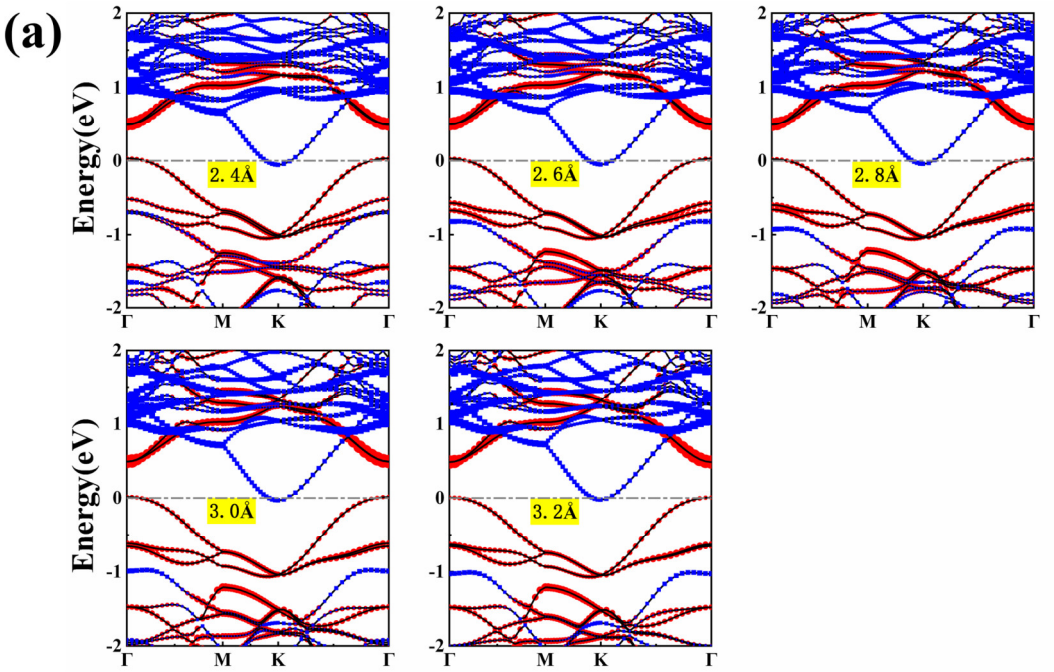
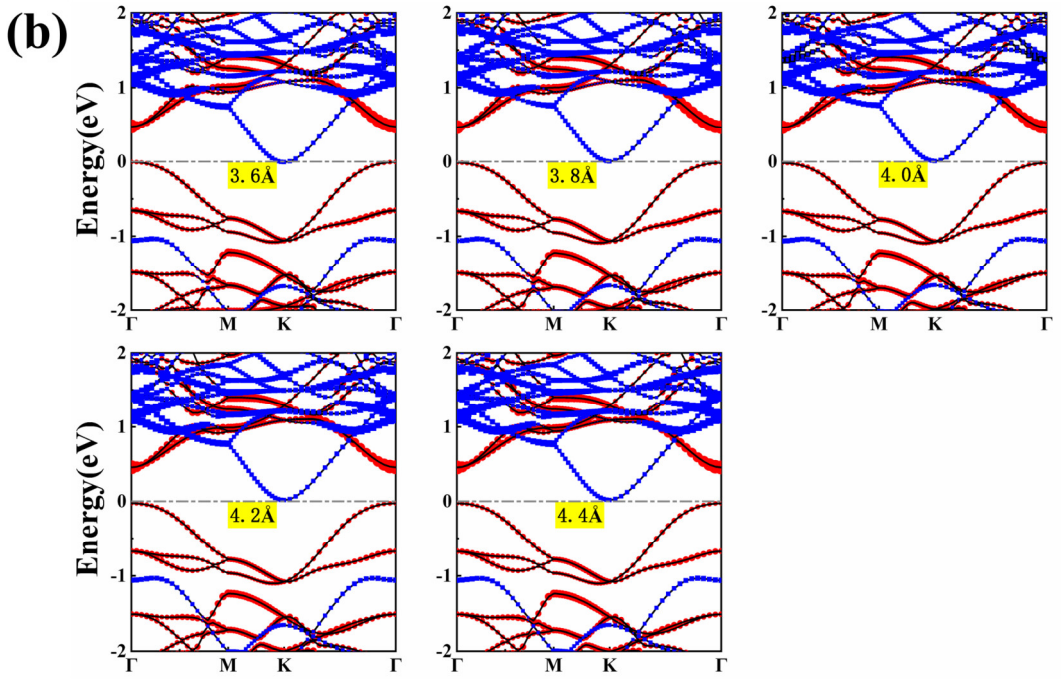
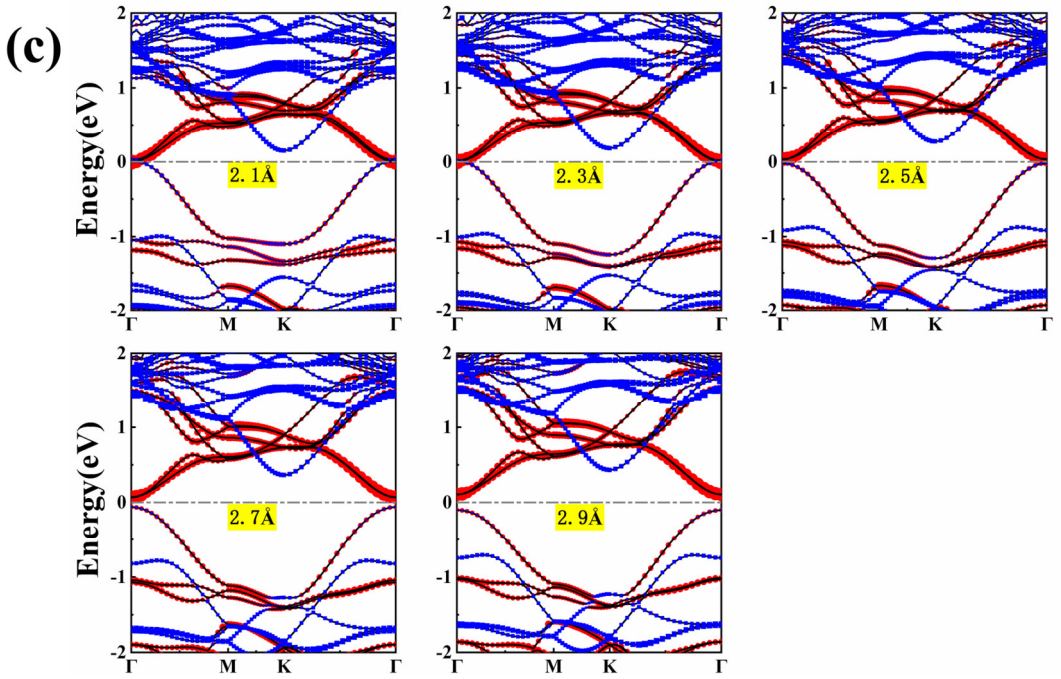


Figure S3. Band structures of (**a**) (**b**) Te_4-MoSTe/$MoGe_2N_4$ vdWH, (**c**) (**d**) S_4-MoSTe/$MoGe_2N_4$ vdWH under biaxial strains. The red and blue represent the weights from Janus MoSTe and $MoGe_2N_4$ monolayers, respectively. Negative and positive values mean compressive stress and tensile stress.




(b)
Energy(eV)
3.6Å
3.8Å
4.0Å
4.2Å
4.4Å
Γ M K Γ


(c)
Energy(eV)
2.1Å
2.3Å
2.5Å
2.7Å
2.9Å
Γ M K Γ

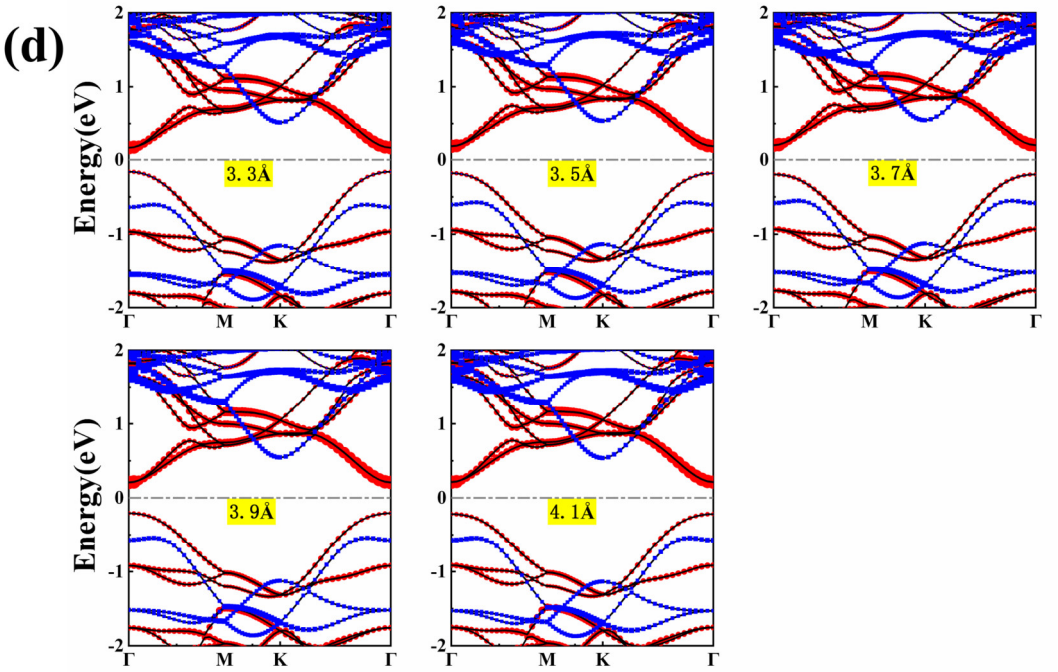


Figure S4. Band structures of (**a**) (**b**) Te_4-MoSTe/$MoGe_2N_4$ vdWH, (**c**) (**d**) S_4-MoSTe/$MoGe_2N_4$ vdWH under different interlayer distances, where the equilibrium interlayer distances are 3.4 Å and 3.1Å, respectively. The red and blue represent the weights from Janus MoSTe and $MoGe_2N_4$ monolayers, respectively. .