Supplementary Materials

Tunable type-I band alignment and electronic structure of GaSe/$MoSi_2N_4$ van der Waals heterostructure

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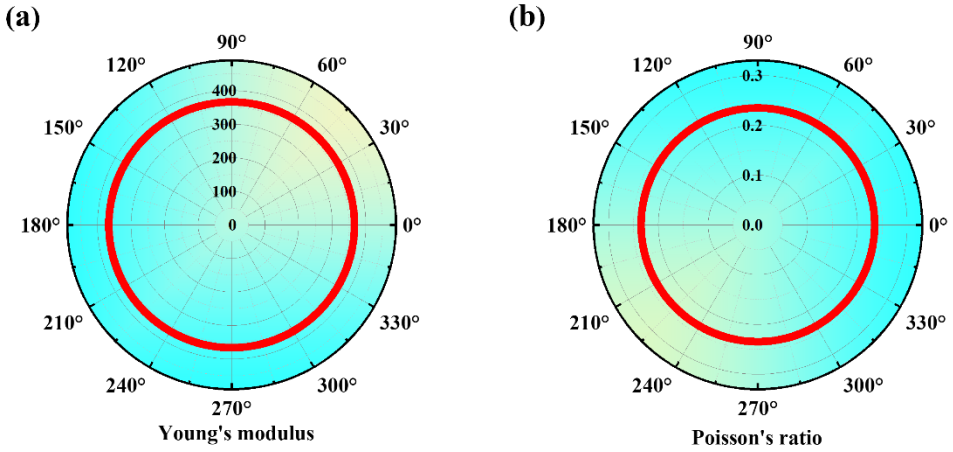

Figure S1. Orientation-dependent (a) Young's modulus and (b) Poisson's ratio for ground state GaSe/$MoSi_2N_4$ vdWHs.

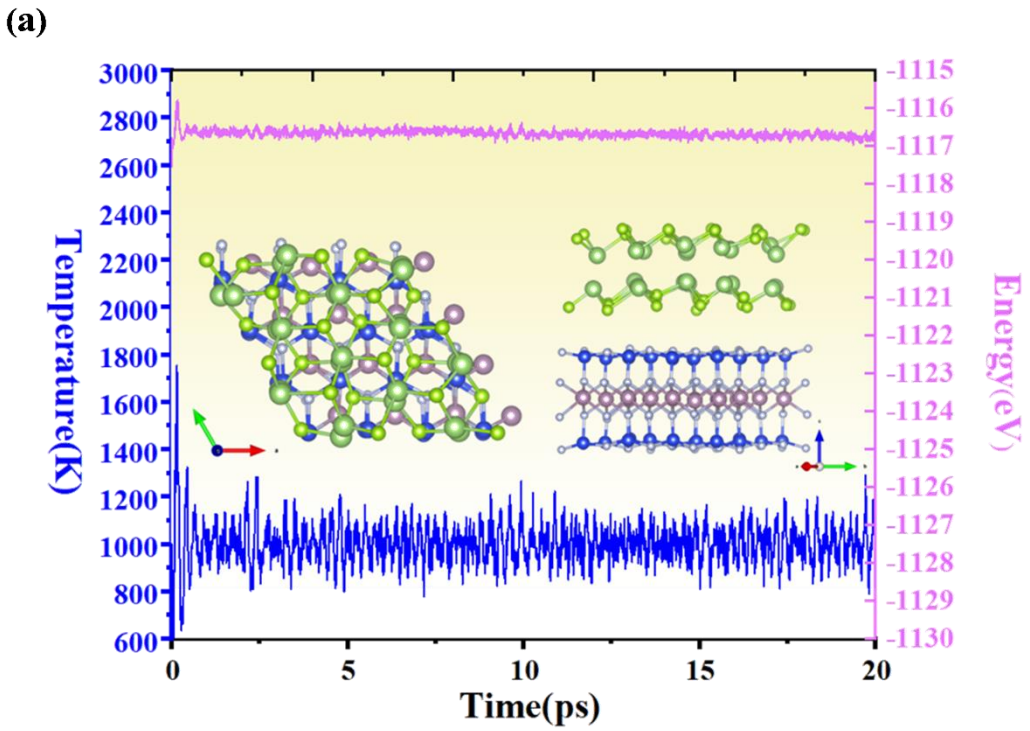

Figure S2. The structure and energy fluctuation of the GaSe/$MoSi_2N_4$ heterostructure at 1000 K.

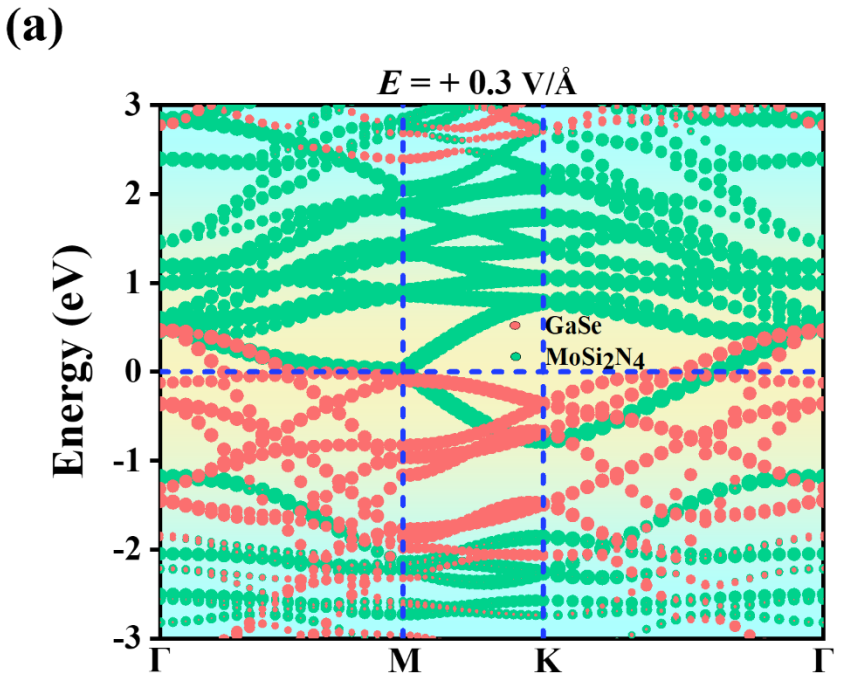

Figure S3. Projected band structure of GaSe/$MoSi_2N_4$ vdWHs at an electric field of +0.3 V/Å. The Fermi level is set to zero. The red and green circles represent the contributions of layers GaSe and $MoSi_2N_4$, respectively.

Table S1. Calculation of binding energy of GaSe/MoSi2N4 heterostructures under modifying the interlayer distance(ΔD) for different stacking modes

ΔD (Å)	Binding Energy (eV)		
stacking modes	AA	AB	AC
-0.6	-7.04537	-7.04391	-7.04681
-0.4	-7.05117	-7.05028	-7.05141
-0.2	-7.05357	-7.05379	-7.05369
0	-7.05358	-7.05376	-7.05395
0.2	-7.05317	-7.05305	-7.05324
0.4	-7.05197	-7.05194	-7.05203