Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Boosting the photocatalytic hydrogen evolution performance of C_2N monolayer coupled with $MoSi_2N_4$: density-functional theory calculations

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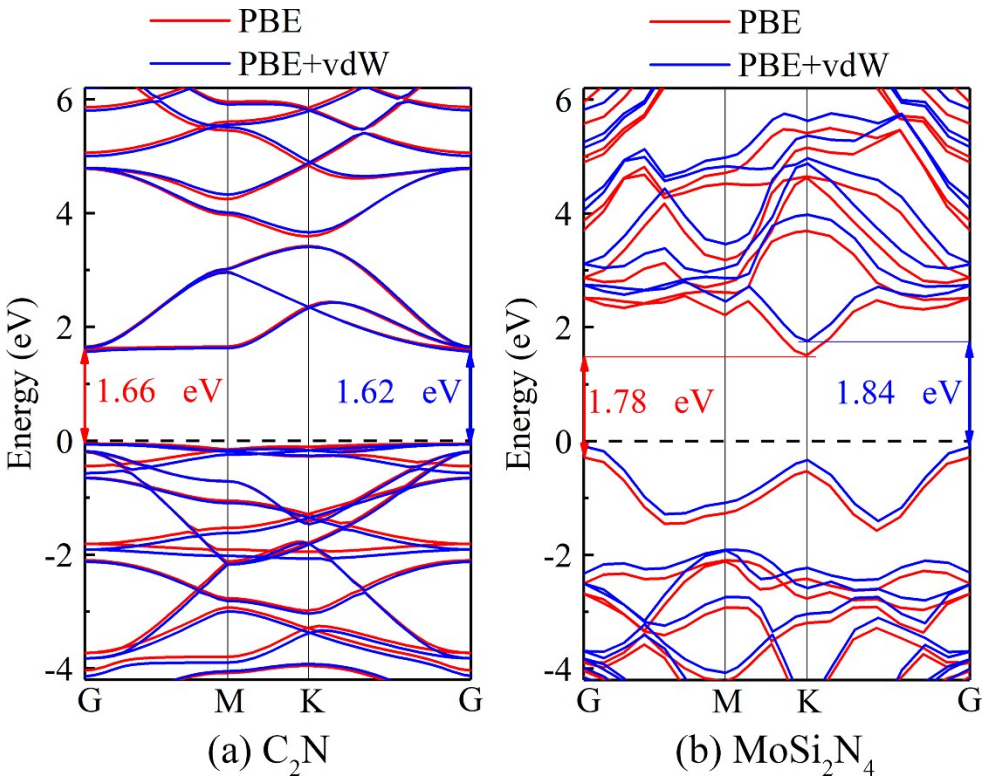

Figure S1. Calculated band structures of (a) C_2N and (b) $MoSi_2N_4$ monolayers with PBE method. The red and blue lines represent the results with and without vdW correction, respectively.

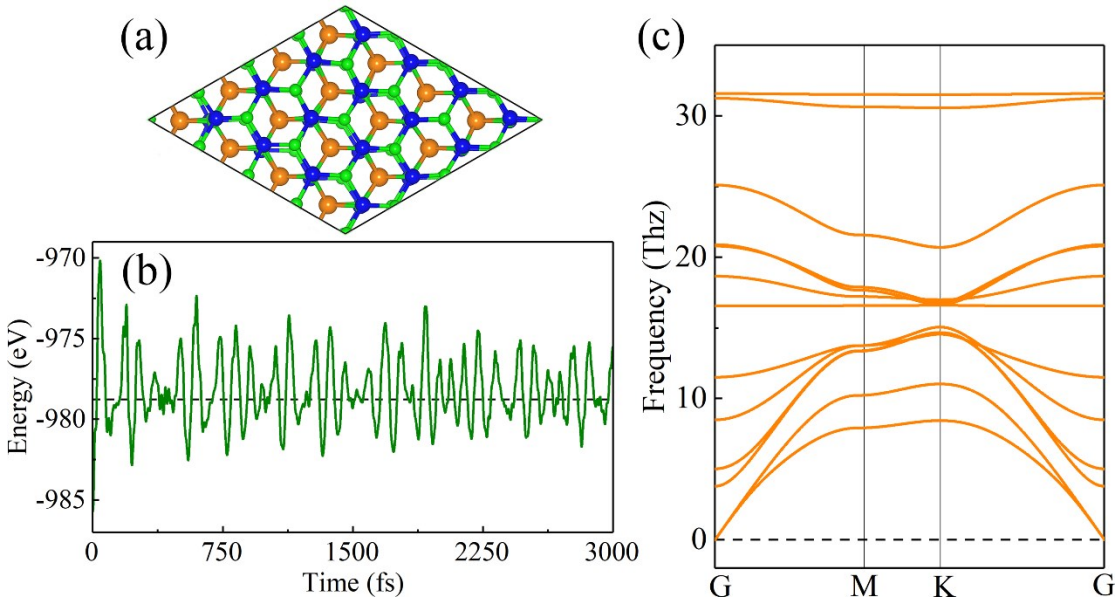

Figure S2. (a) Top view of the snapshot from the molecular dynamics simulation of atomic structures for 4×4 $MoSi_2N_4$ at 300 K. (b) Variation of the total potential energy in the molecular dynamics simulation at room temperature during the time scale of 3.0 ps. (d) The calculated phonon dispersion spectra of $MoSi_2N_4$.

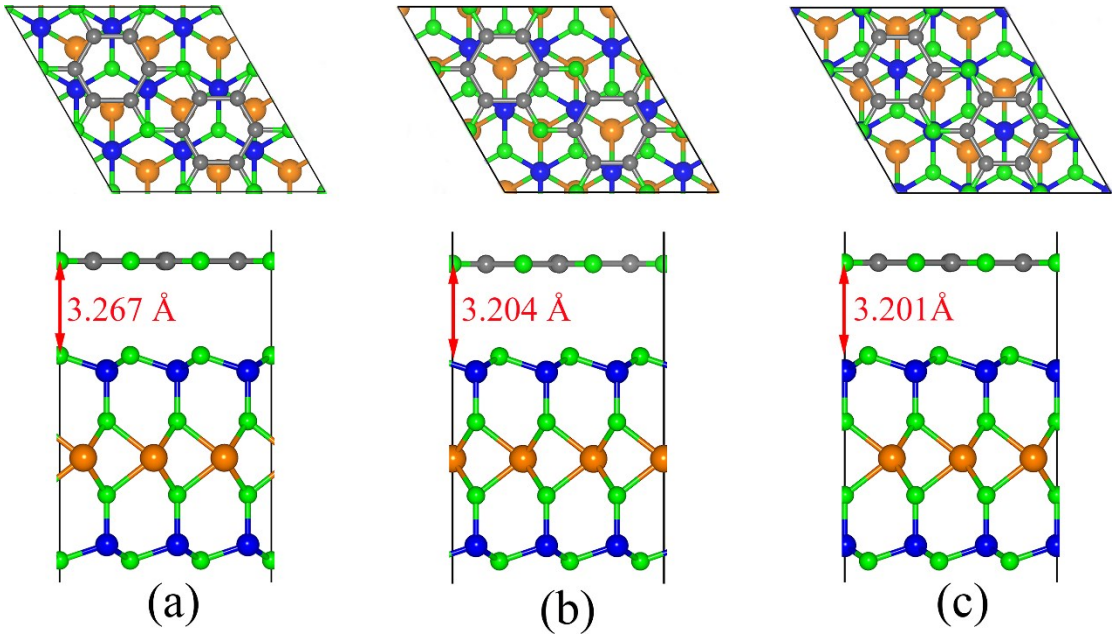

Figure S3. Three different stacking patterns for $C_2N/MoSi_2N_4$ heterojunctions with high symmetry, including top and side views.

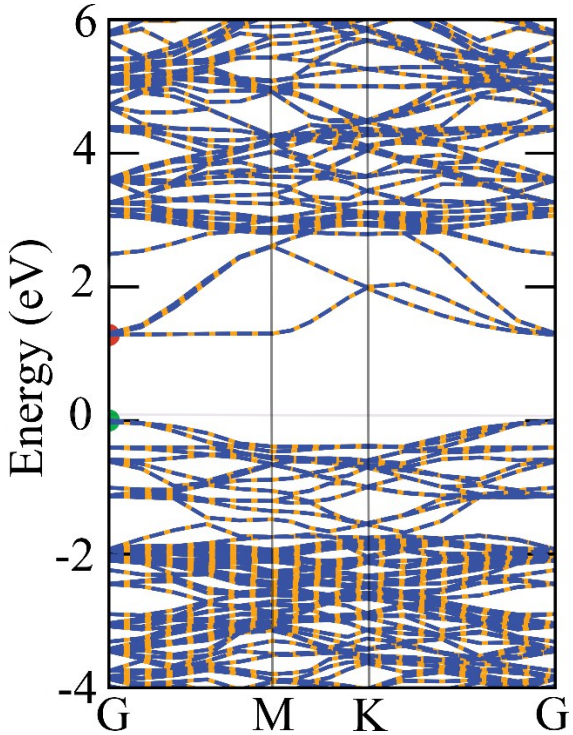

Figure S4. Spin polarized band of $C_2N/MoSi_2N_4$ heterojunction using PBE calculation.