Supplementary Information

Tunable type-II lateral $MoSi_2N_4/WSi_2N_4$ heterostructures for photocatalytic applications

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Table I. The detailed information about crystal structure in $(MoSi_2N_4)_m(WSi_2N_4)_n$ lateral HSs with different widths. The w, a, h and S are the width, lattice constant, thickness and contact area of lateral HSs, respectively.

m(n)	w (Å)	a (Å)	h (Å)	S (Å^2)
4(4)	10. 563	5. 029	7. 060	35. 504
5(5)	13. 479	5. 033	7. 068	35. 575
6(6)	16. 396	5. 035	7. 071	35. 603
7(7)	19. 304	5. 036	7. 073	35. 622
8(8)	22. 216	5. 038	7. 073	35. 630

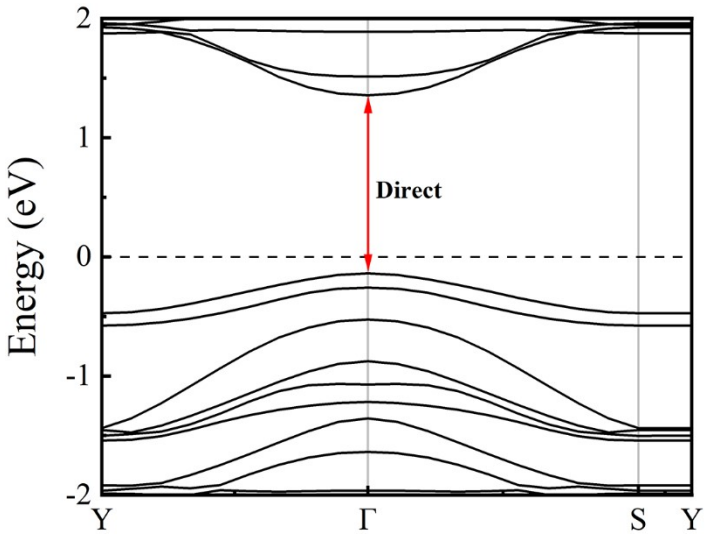

Fig. S1. Band structure of $(MoSi_2N_4)_4(WSi_2N_4)_4$ lateral heterostructure based on HSE

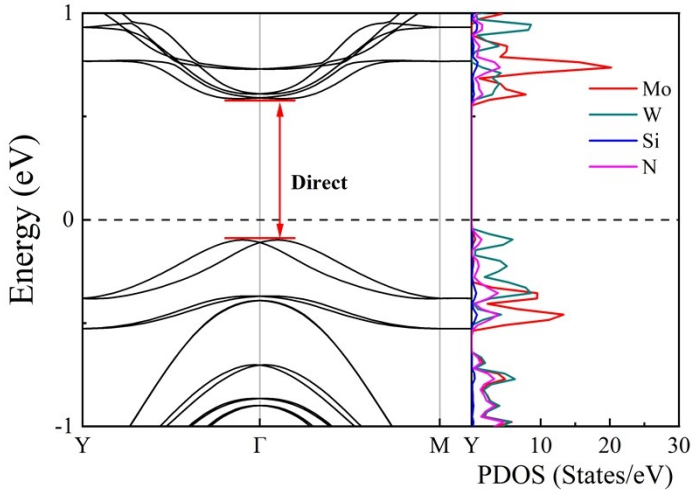

Fig. S2. Band structure and PDOS of $(MoSi_2N_4)_5(WSi_2N_4)_5$ based on PBE+SOC.

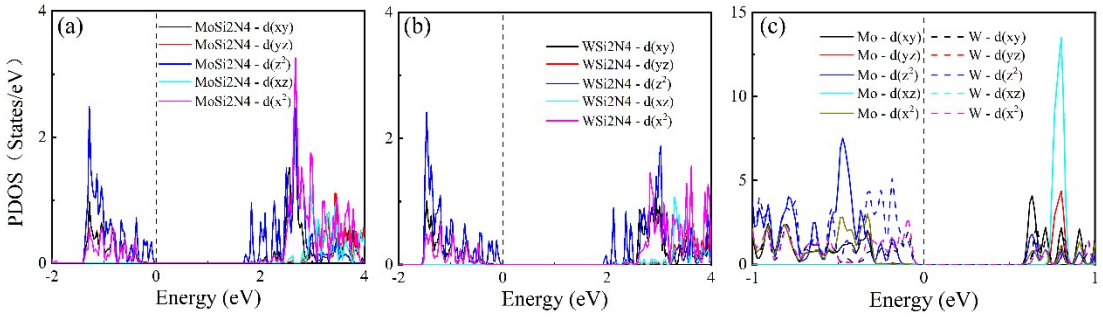

Fig. S3. The density of states of d orbitals of Mo/W in the (a) $MoSi_2N_4$, (b) $MoSi_2N_4$ and (c) $(MoSi_2N_4)_8(WSi_2N_4)_8$ lateral HSs.

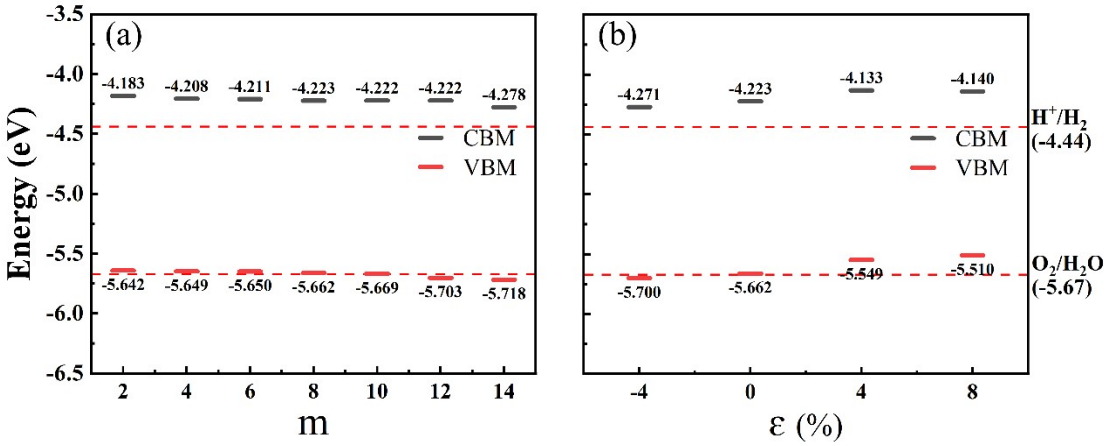

Fig. S4. The band alignments of (a) $(MoSi_2N_4)_m(WSi_2N_4)_n$ (m+n=16) with the different component ratios, (b) $(MoSi_2N_4)_8(WSi_2N_4)_8$ lateral HSs with the different strains.