Electronic supplementary information (ESI)

High hydrogen production in InSe/$MoSi_2N_4$ van der Waals heterostructure for overall water splitting

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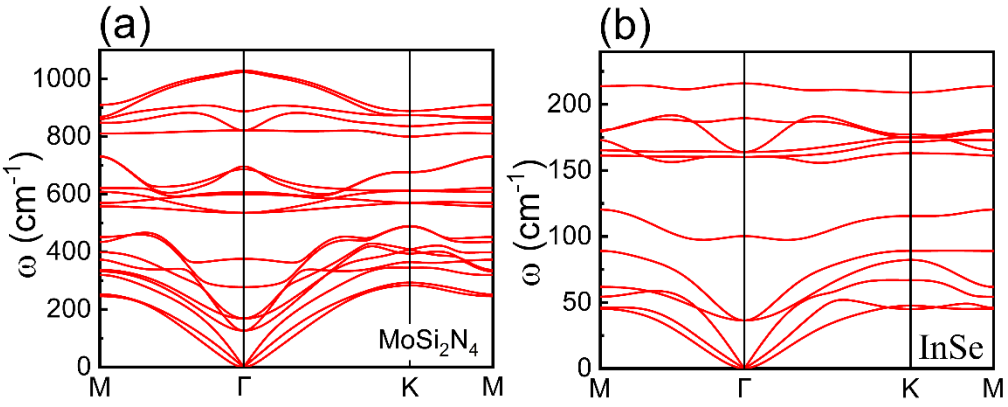

Fig. S1 Calculated phonon spectra of (a) $MoSi_2N_4$ and (b) InSe layers, respectively.

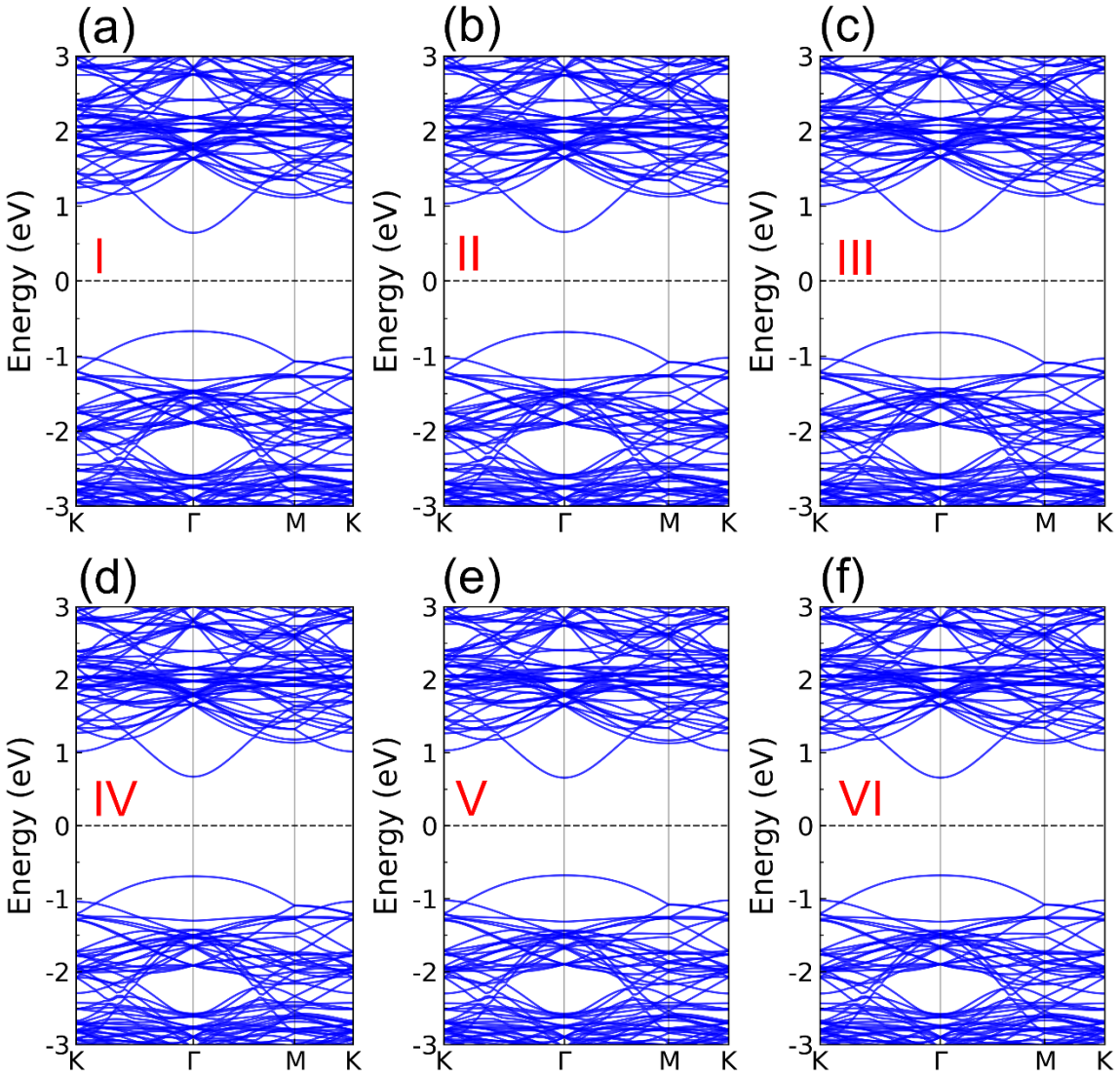

Fig. S2 Calculated band structures (PBE method) of six different stacking configurations for InSe/$MoSi_2N_4$ heterostructures.

Table S1 The lattice constants a/b, interlayer distance d, buckling height of InSe h_1 and $MoSi_2N_4$ h_2, formation energy E_f and band gap E_g^{PBE} of InSe/$MoSi_2N_4$ heterostructure

	a/b (Å)	d (Å)	h_1 (Å)	h_2 (Å)	E_f (meV/atom)	E_g^{PBE} (eV)
I	10.480	3.311	5.429	6.993	-14.965	1.342
II	10.479	3.284	5.426	6.992	-15.012	1.335
III	10.480	3.326	5.460	6.991	-15.005	1.352
IV	10.479	3.282	5.445	6.980	-15.000	1.365
V	10.480	3.293	5.452	6.993	-14.975	1.338
VI	10.479	3.286	5.455	6.974	-15.022	1.339