Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information for

A type-II blue phosphorus/$MoSe_2$ van der Waals heterostructure: improved electronic and optical properties via vertical electric field

Huabing Shu*

School of Science, Jiangsu University of Science and Technology, Zhenjiang 212001, China

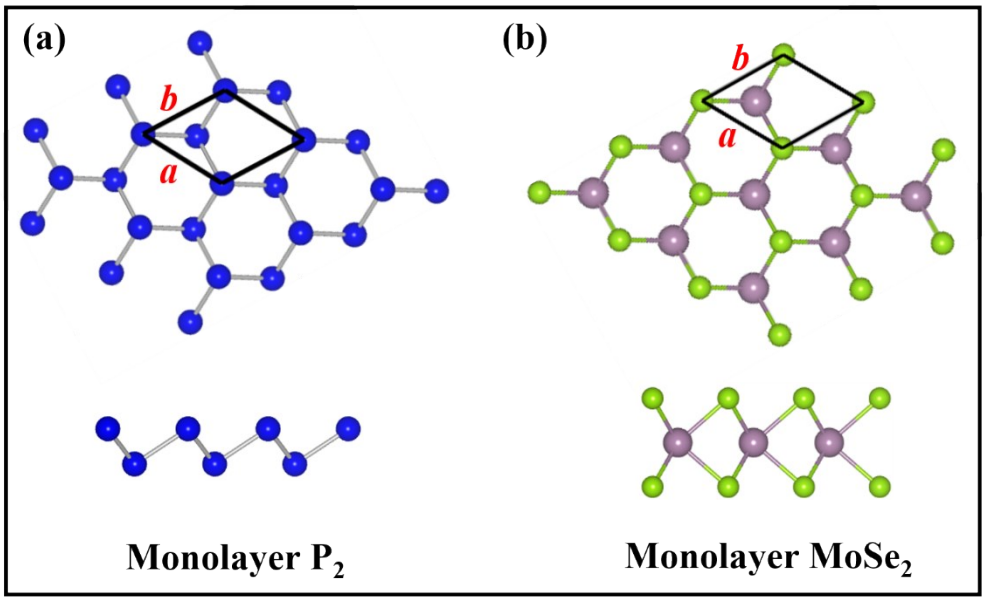

Fig. S1 The optimized configurations of the P_2 (a) and $MoSe_2$ (b) monolayers. The P atom, Se atom, and Mo atom are denoted by blue sphere, green sphere, and purple sphere, respectively.

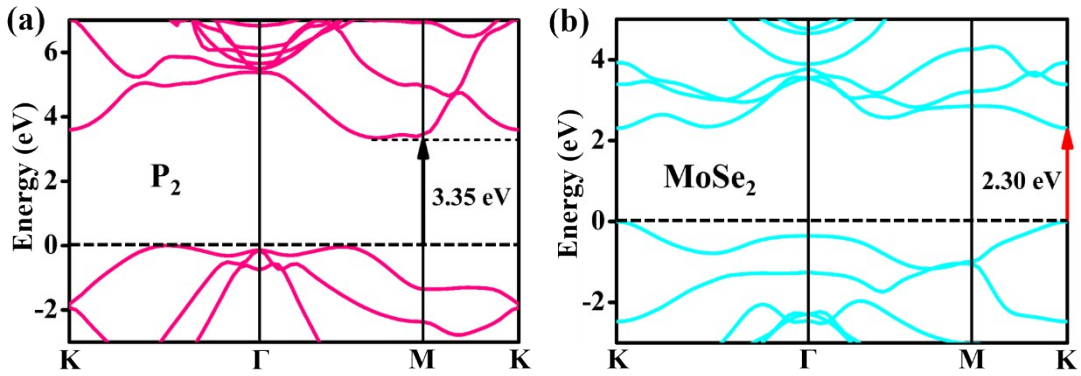

Fig. S2 Quasi-particle band structures of the P_2 (a) and $MoSe_2$ (b) monolayers computed by the single-shot G_0W_0 method. The valence band maximum is shifted to zero.

Table S1 Structural parameters and formation energies of the $P_2/MoSe_2$ vdW heterostructures: lattice constants (a/b), bond lengths (l), interlayer distances (d), formation energies (E_f).

Type	a/b (Å)	$l_{P\text{-}P}$ (Å)	$l_{Mo\text{-}Se}$ (Å)	d (Å)	E_f (eV/unit)
AA-I	3.291	2.270	2.535	3.697	–0.212
AA-II	3.296	2.275	2.569	3.799	–0.201
AB-I	3.294	2.270	2.537	3.852	–0.185
AB-II	3.288	2.269	2.535	3.809	–0.191
AB-III	3.289	2.276	2.570	3.703	–0.208

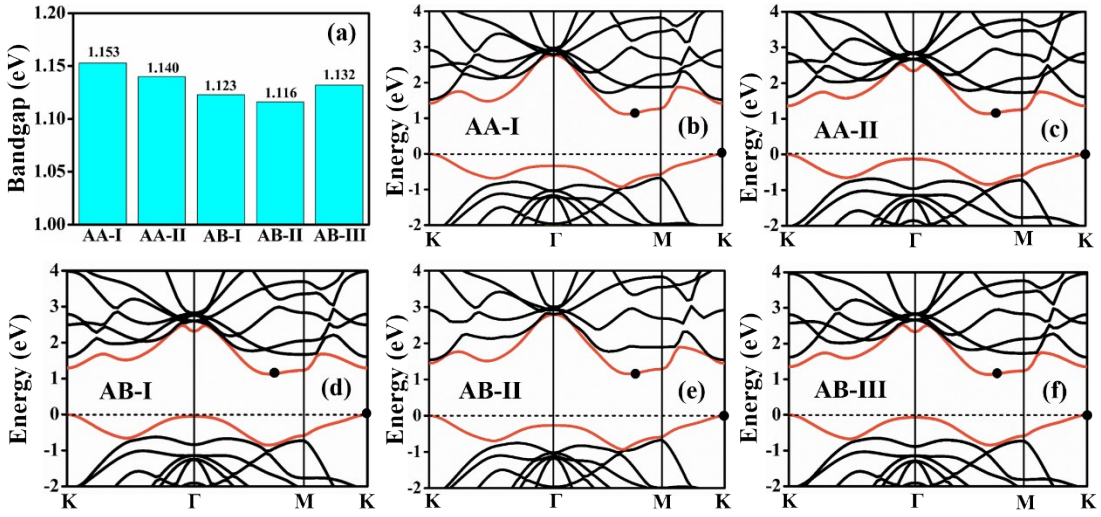

Fig. S3 Variable bandgaps (a) and band structures (b)-(f) of the $P_2/MoSe_2$ vdW heterostructures with different stacking configurations at the PBE level.

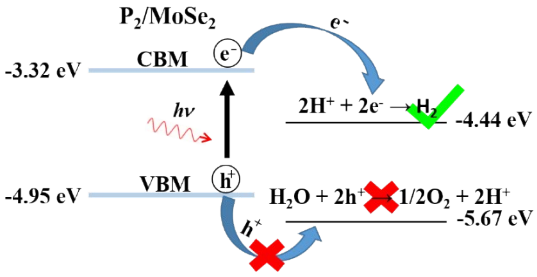

Fig. S4 Illustration of photocatalytic water splitting of the $P_2/MoSe_2$ vdW heterostructure at pH = 0.

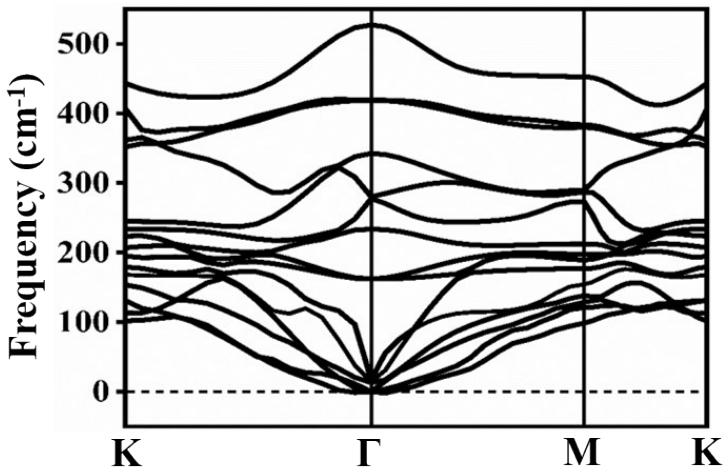

Fig. S5 Phonon spectra of $P_2/MoSe_2$ vdW heterostructure at the electric field of 0.4 V/Å.

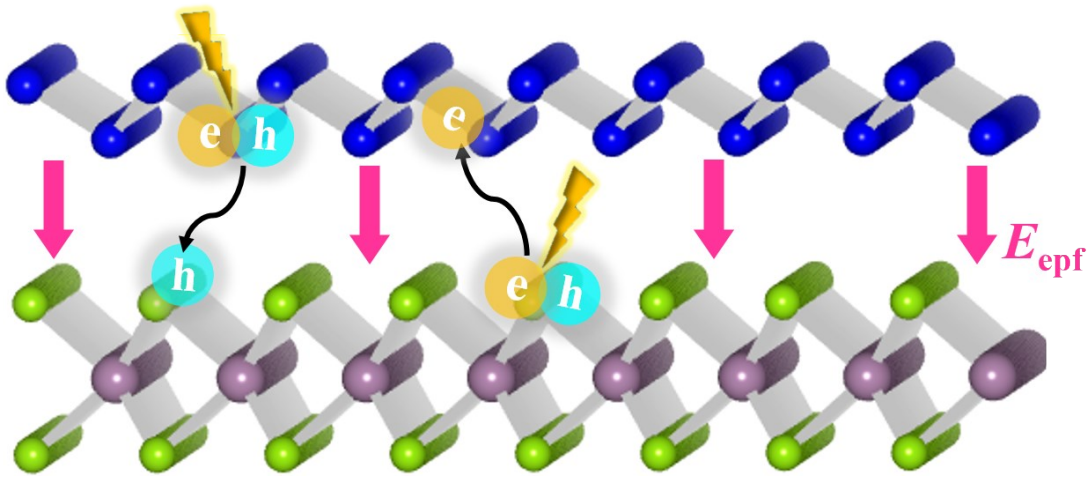

Fig. S6 Schematic diagram of the separation of photoexcited electrons and holes on the interface under the electric polarized field.

Table S2 Bader charge transfer (Δq) and electric polarized field (E_{epf}) between the P_2 layer and $MoSe_2$ layers induced by vertical electric field (E_{ef}). The positive value of the Δq show the charges transfer from the P_2 layer to $MoSe_2$ layer. The negative value of the E_{epf} denotes the direction pointed from the P_2 layer to $MoSe_2$ layer. Units of the charge and electric field are 10^{-2} e and V/Å, respectively.

E_{ef}	-0.40	-0.30	-0.20	-0.10	0	0.10	0.20	0.30	0.40
Δq	-0.12	0.04	0.19	0.33	0.49	0.63	0.81	0.98	1.15
E_{epf}	0.023	-0.007	-0.037	-0.064	-0.094	-0.121	-0.156	-0.189	-0.222

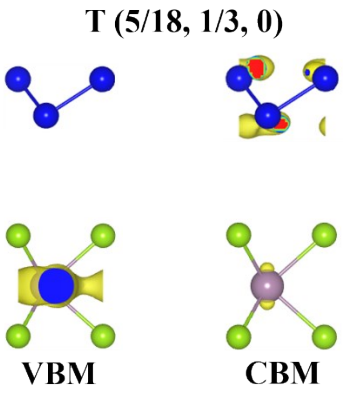

Fig. S7 Decomposed charge density of the CBM and VBM at **T** point for the $P_2/MoSe_2$ vdW heterstructure. Isosurface is set to 3.0×10^{-3} e/Å^3.