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

Supplementary Data

First-principles study of two-dimensional $NbSe_2H$/g-ZnO van der Waals heterostructures as a water splitting photocatalyst

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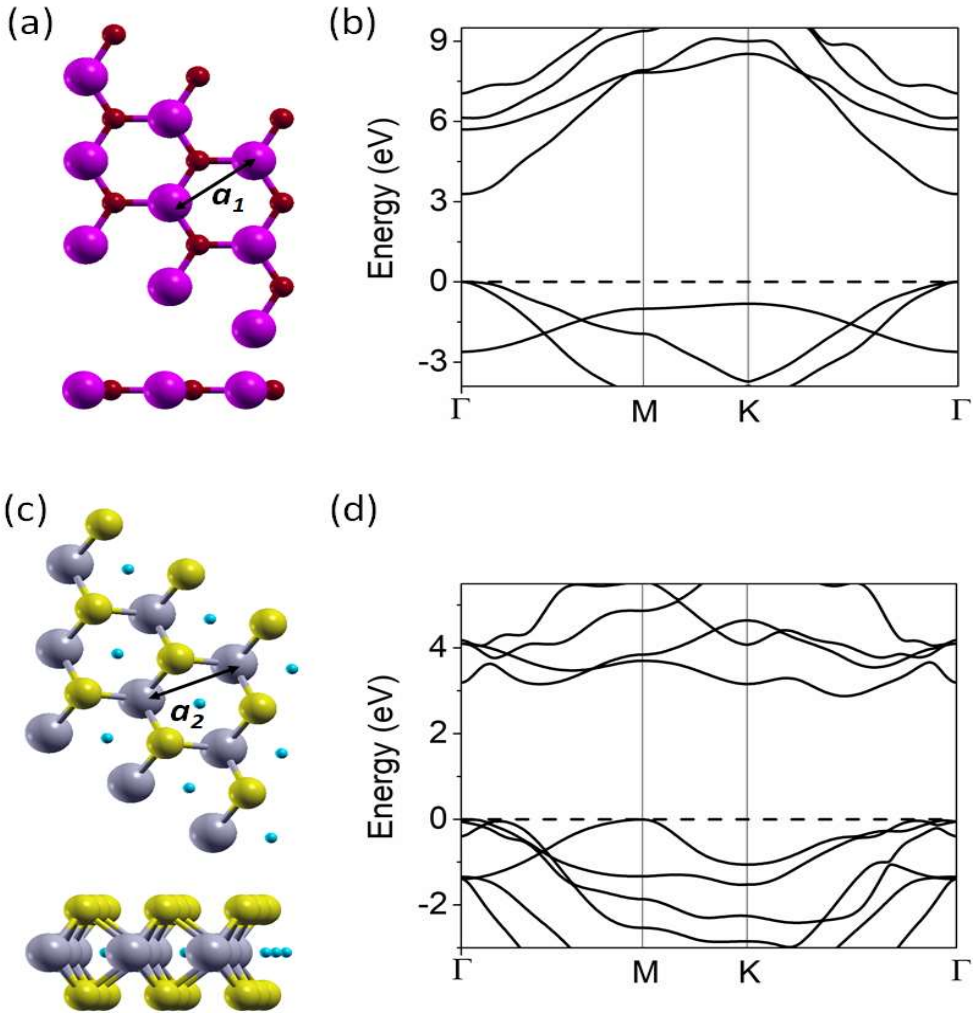

Fig. S1: Top and side views of the crystal structure for (a) g-ZnO and (c) 2D $NbSe_2H$. The band structures for (b) g-ZnO and (d) 2D $NbSe_2H$ were calculated by using HSE06 functional. The lattice constant for the g-ZnO and 2D $NbSe_2H$ are denoted by $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$, respectively.

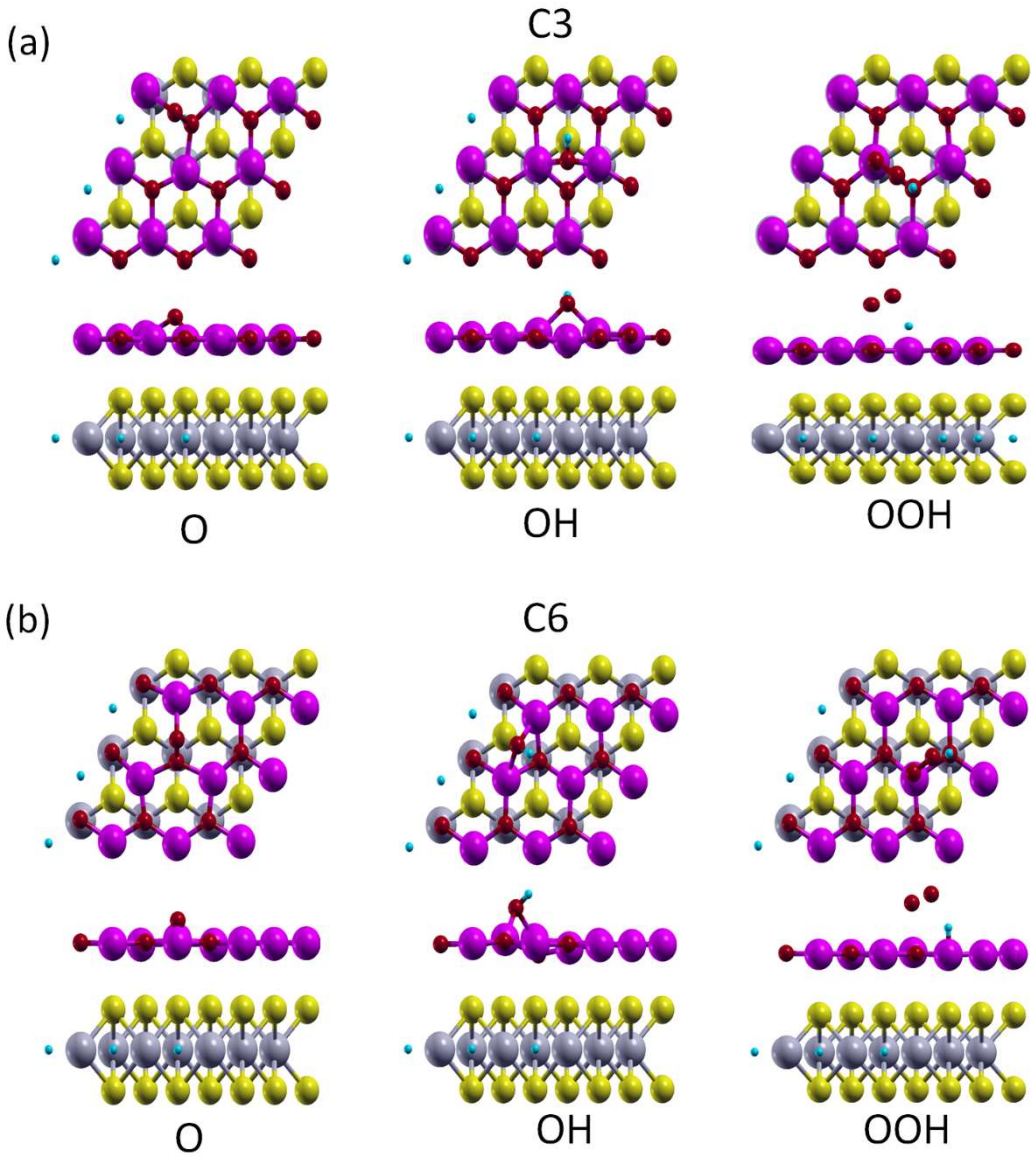

Fig. S2: Adsorption of O, OH and OOH intermediates on the $NbSe_2H$/g-ZnO vdW heterostructures for (a) C3 and (b) C6 stackings. Yellow, grey, cyan, purple, and red balls denote Se, Nb, H, Zn and O atoms, respectively.

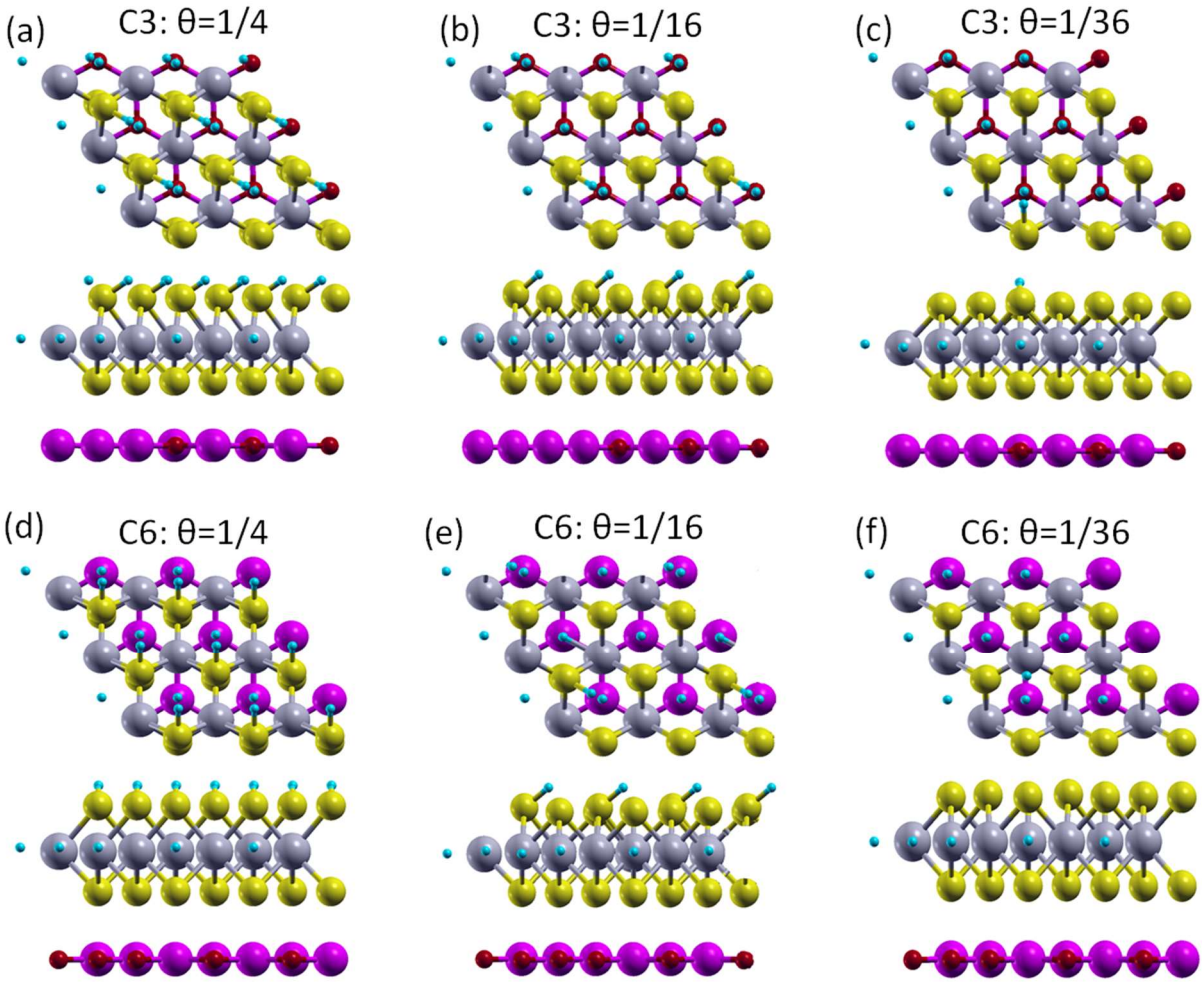

Fig. S3: Adsorption of H on the surface of 2D $NbSe_2H$ in the $NbSe_2H$/g-ZnO vdW heterostructures. The coverage of the H atoms are $\theta = 1/4$ for (a) C3 and (d) C6 stackings, $\theta = 1/16$ for (b) C3 and (e) C6 stackings and $\theta = 1/36$ for (c) C3 and (f) C6 stackings Yellow, grey, cyan, purple, and red balls denote Se, Nb, H, Zn and O atoms, respectively.