

**Supporting information:**

**Effects of doping on photocatalytic water splitting activities  
of PtS<sub>2</sub>/SnS<sub>2</sub> van der Waals heterostructure**

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**Table S1** The under table shows the crystallographic information and the calculated lattice parameters of PtS<sub>2</sub> and SnS<sub>2</sub> monolayers.

Compound	PtS <sub>2</sub>	SnS <sub>2</sub>
Crystal system	hexagonal	hexagonal
a (Å)	3.572	3.699
b (Å)	3.572	3.699
$\alpha$ (°)	90	90
$\beta$ (°)	90	90
$\gamma$ (°)	120	120
reference data (Å)	a=b=3.55 <sup>1</sup>	a=b=3.698 <sup>2</sup>

1. S. U. Rehman, B. Amin, M. Hafeez, S. A. Khan, I. A. Mir, W. Uddin, L. Wei and L. Zhu, *Appl. Surf. Sci.*, 2020, **505**, 144530.
2. C. Xia, J. Du, M. Li, X. Li, X. Zhao, T. Wang and J. Li, *Phys. Rev. Appl.*, 2018, **10**.

Fig. S1 Energy tests of PtS<sub>2</sub>/SnS<sub>2</sub> vdWHs for interlayer spacing (a) and density of k-mesh (b).

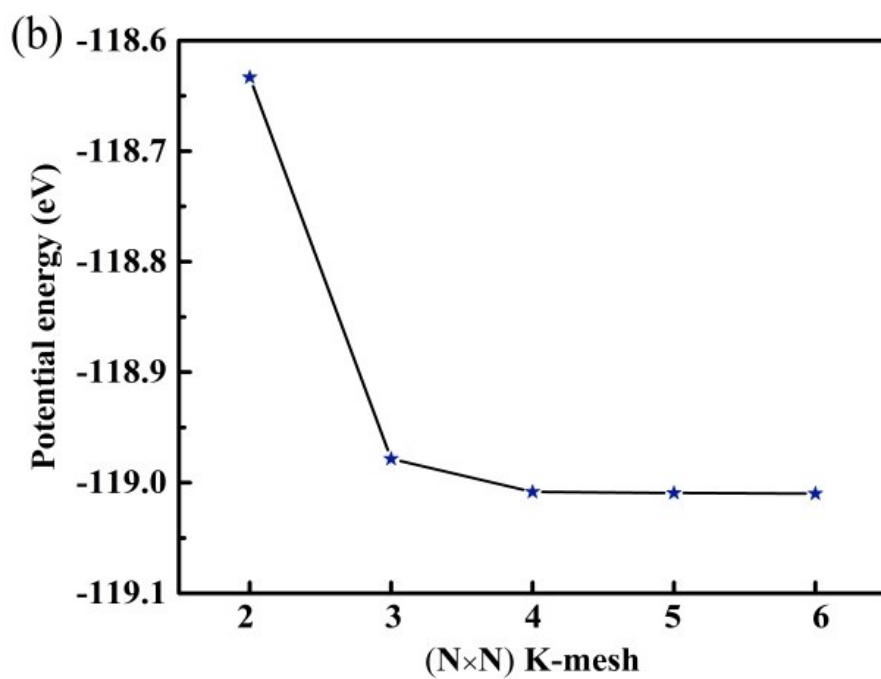
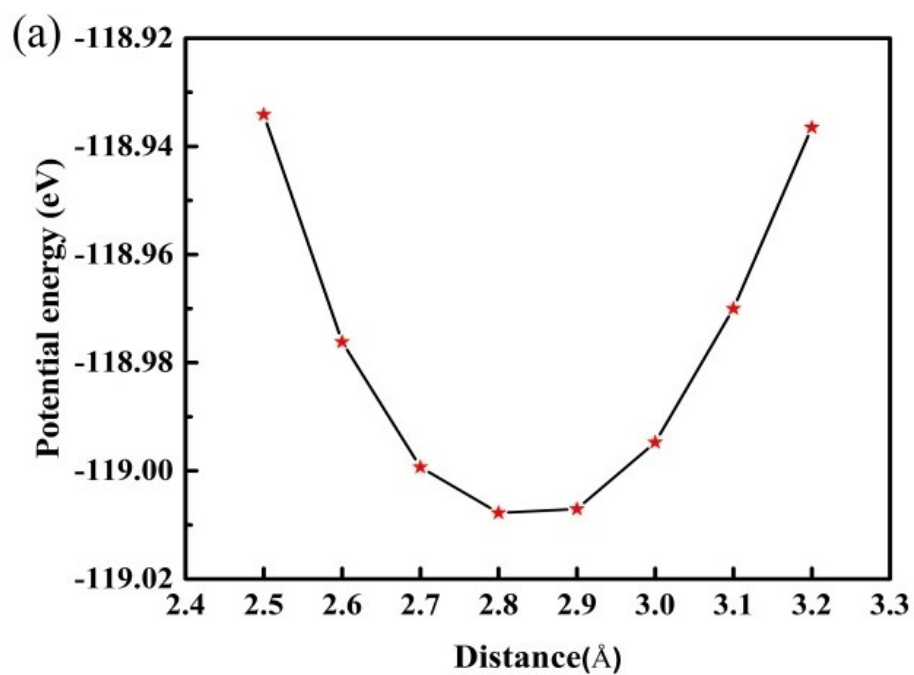


Fig. S2 (a) calculated phonon spectrum of PtS<sub>2</sub>/SnS<sub>2</sub> vdW heterojunction. (b) free energy changes with simulated time in the AIMD trajectory in PtS<sub>2</sub>/SnS<sub>2</sub> vdW heterojunction.

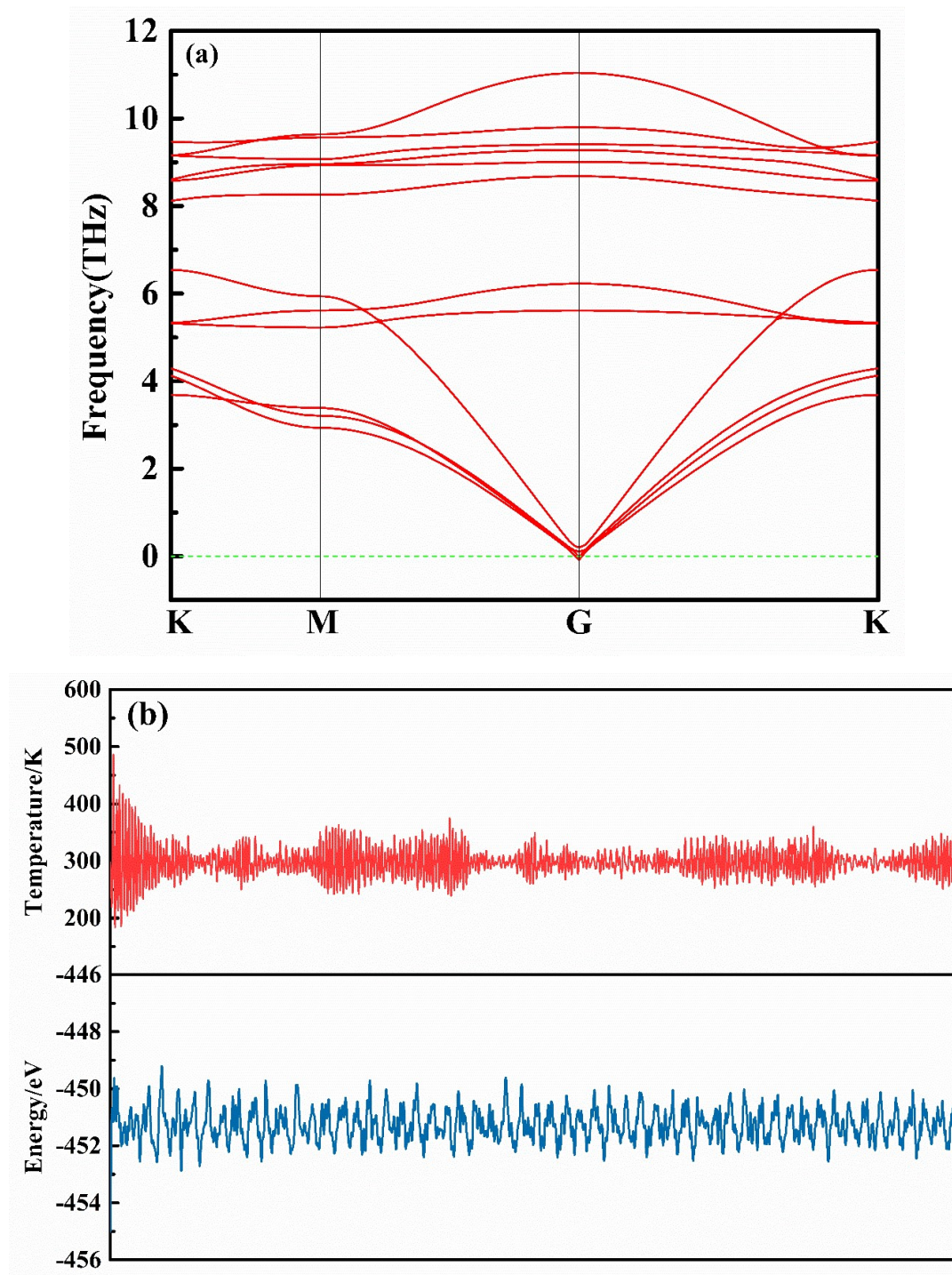
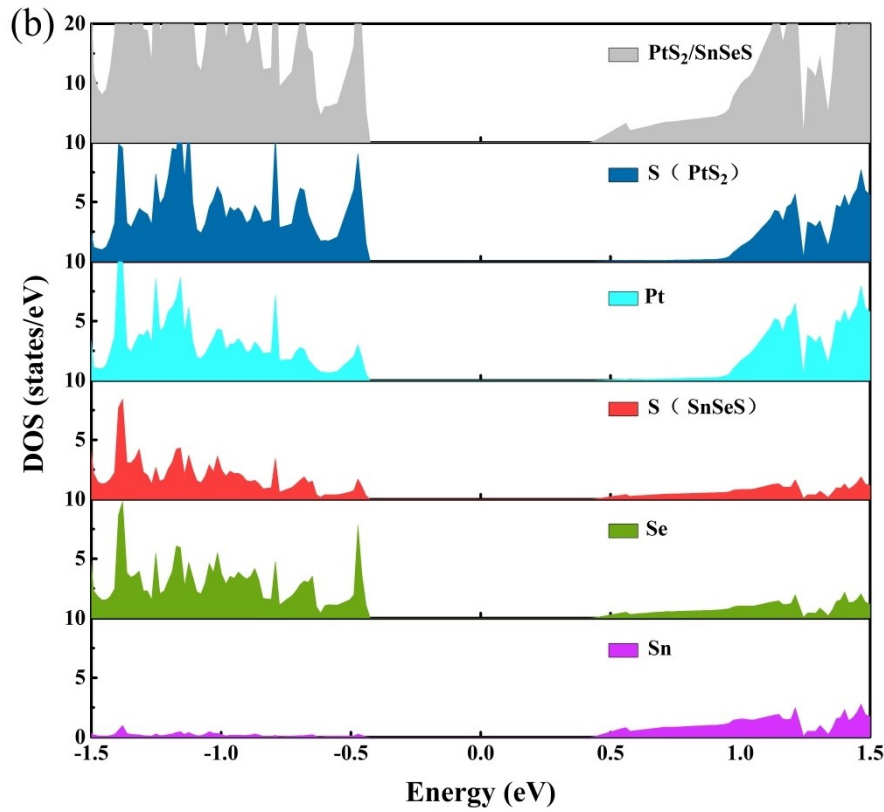
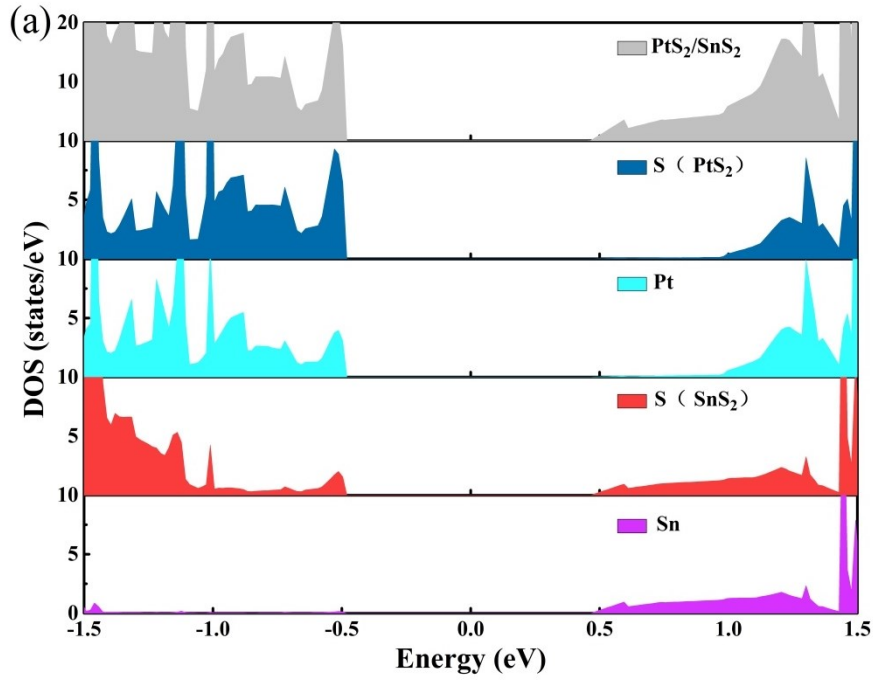
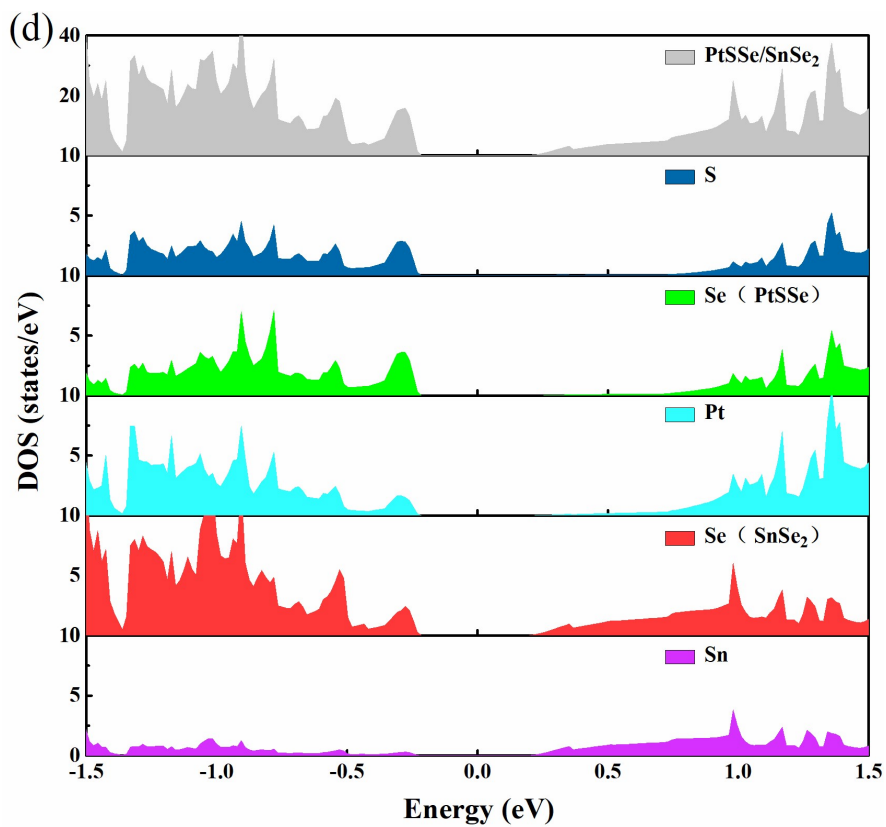
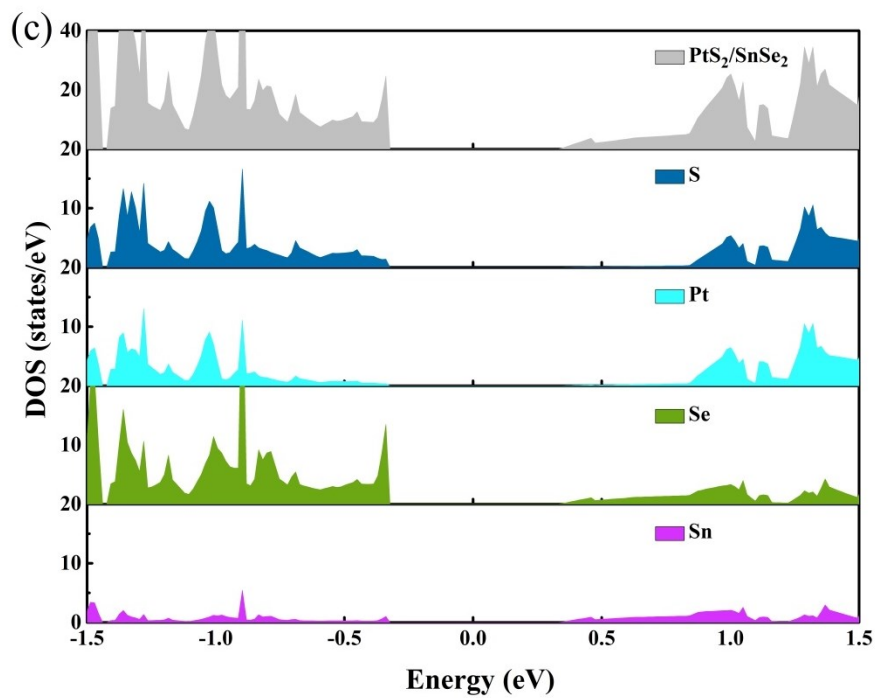


Fig. S3 Calculated density of states (DOS) of (a)PtS<sub>2</sub>/SnS<sub>2</sub>, (b)PtS<sub>2</sub>/SnSSe, (c) PtS<sub>2</sub>/SnSe<sub>2</sub>, (d) PtSSe/SnSe<sub>2</sub>, and (e) PtSe<sub>2</sub>/SnSe<sub>2</sub> vdWHs. The Fermi level is set at 0 eV.





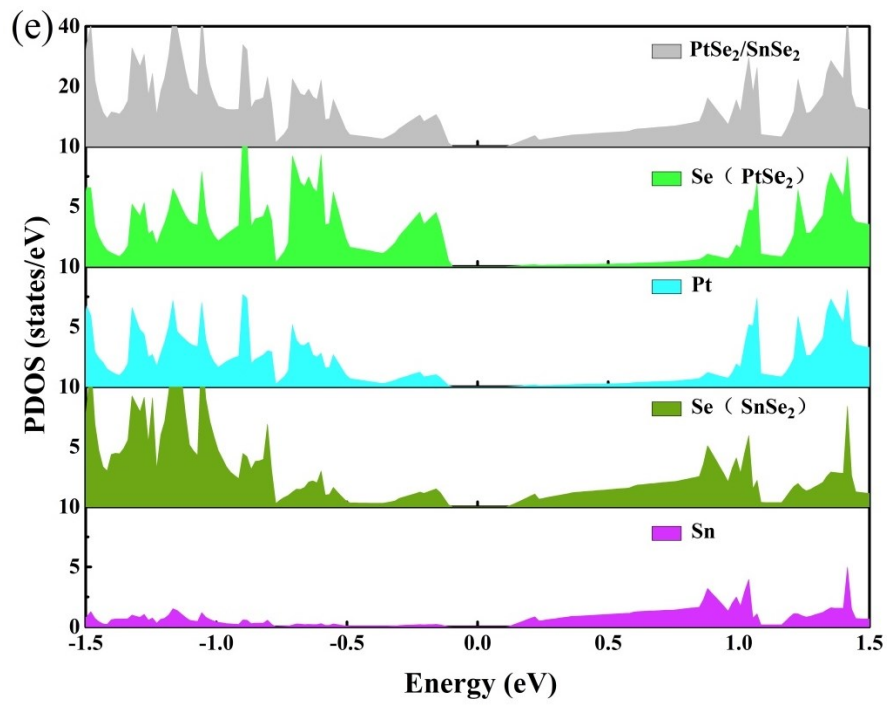


Fig. S4 optical absorption spectra of (a) PtSe<sub>2</sub> monolayer and SnSe<sub>2</sub> monolayer

