

## Supporting information

### **Theoretical Investigation of Arsenene/g-C<sub>6</sub>N<sub>6</sub> Van Der Waals**

#### **Heterojunction: Direct Z-Scheme with High Photocatalytic Efficiency**

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Fig. S1: The diagram of the variation of hydrogen adsorption energy under biaxial strain ranging from -6% to +6%

Fig. S2: The diagram of adsorption intermediates for HER

Fig. S3: The diagram of adsorption intermediates for OER

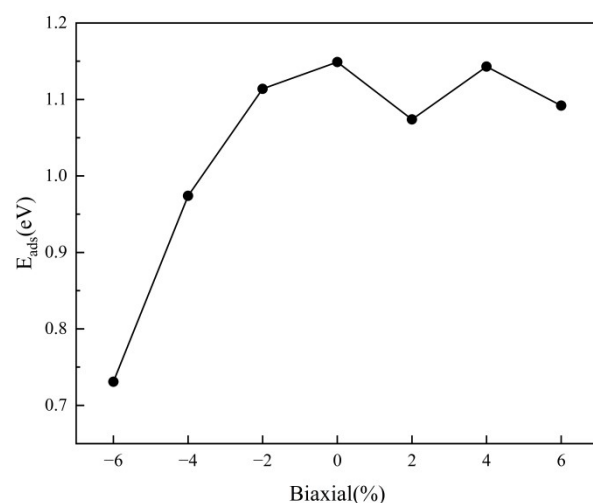


Fig. S 1 Variation of hydrogen adsorption energy under biaxial strain ranging from -6% to +6%. (positive E<sub>ads</sub> values indicate non-spontaneous adsorption, requiring external energy)

HER is conducted at arsenene layer and OER at g-C<sub>6</sub>N<sub>6</sub> layer. Fig. S2 and Fig. S3 show the detailed diagrams of adsorption intermediates for HER and OER,

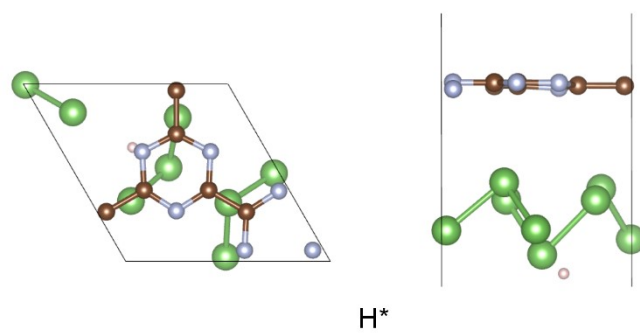


Fig. S 2 The diagram of adsorption intermediates for HER

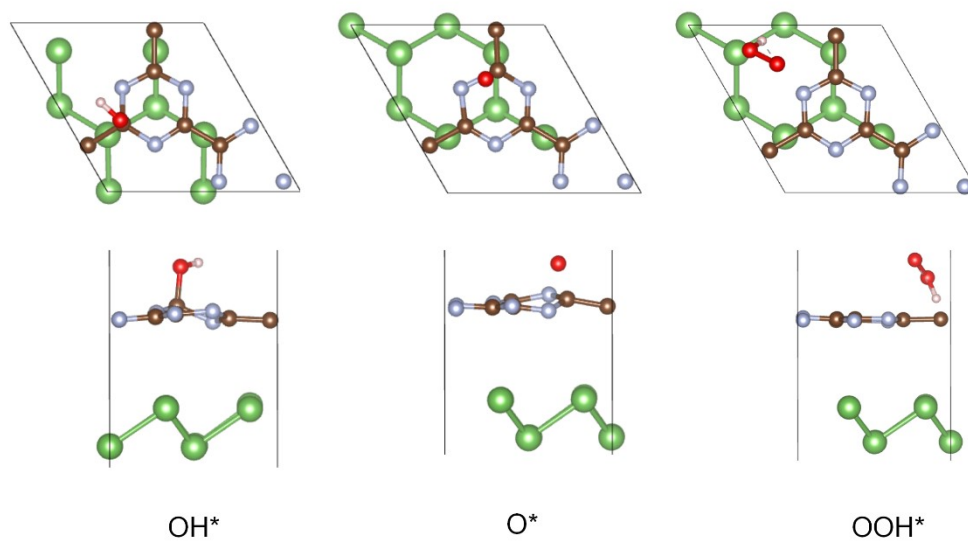


Fig. S 3 The diagram of adsorption intermediates for OER