

*Supplementary Information for*

**The polarized electric field of CdTe/B<sub>4</sub>C<sub>3</sub> heterostructure efficiently  
promote its photocatalytic Overall Water Spitting**

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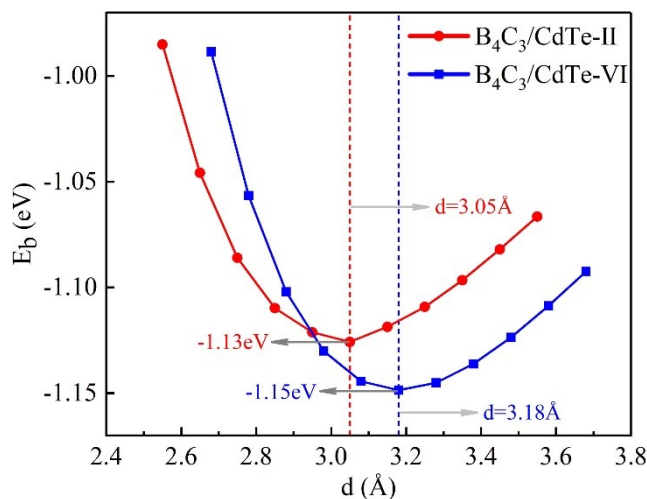


Figure S1 The  $E_b$  curve of CdTe/B<sub>4</sub>C<sub>3</sub>-II and CdTe/B<sub>4</sub>C<sub>3</sub>-V heterostructures as function of interlayer distance  $d$ .

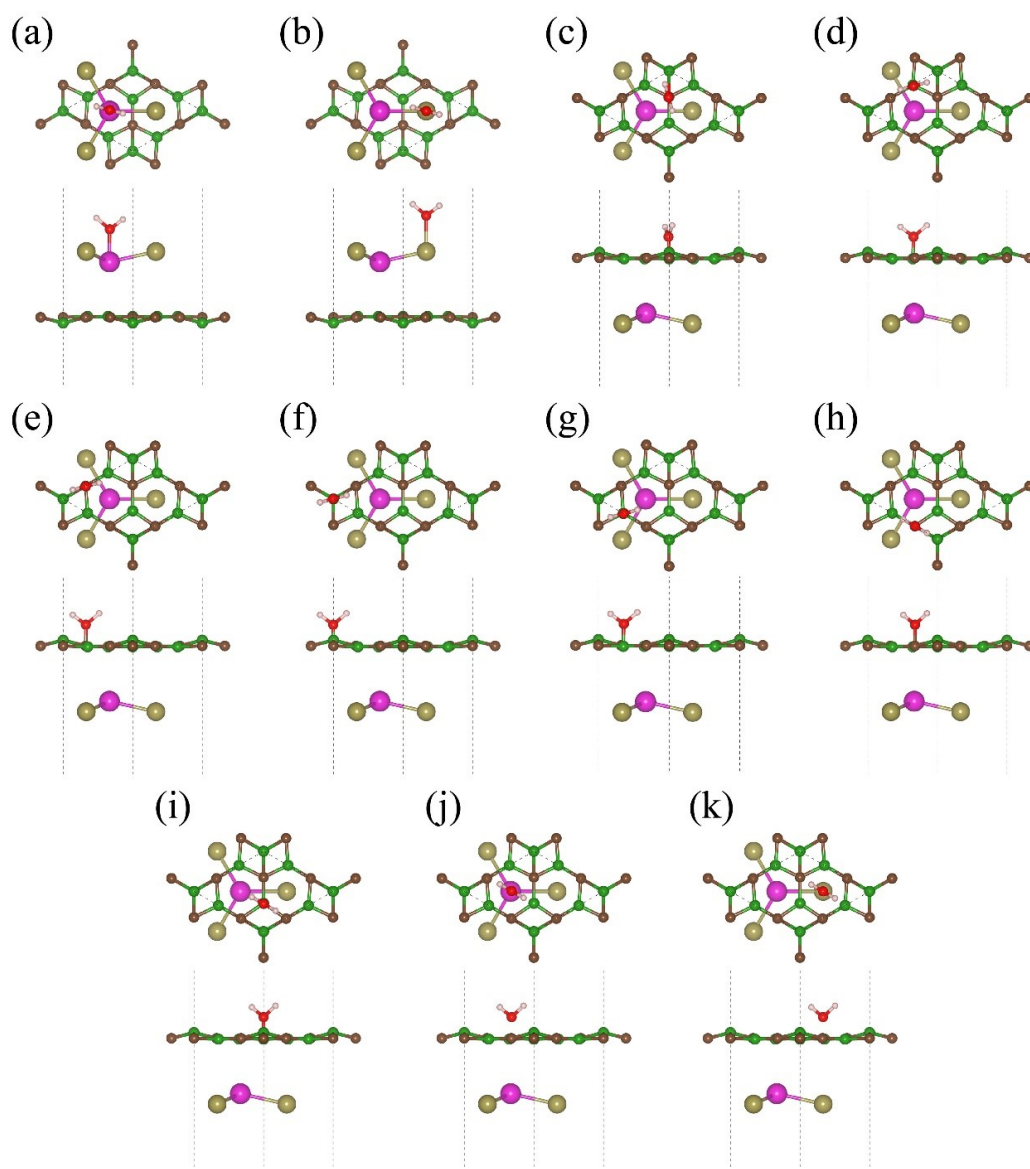


Figure S2 The adsorption configurations of H<sub>2</sub>O molecules in the CdTe/B<sub>4</sub>C<sub>3</sub>-V heterostructure.

Table S2 Adsorption energy of water molecules at different adsorption sites.

Structure	$E(\text{B}_4\text{C}_3/\text{CdTe})/\text{eV}$	$E(\text{H}_2\text{O})/\text{eV}$	$E(\text{B}_4\text{C}_3/\text{CdTe}-\text{H}_2\text{O})/\text{eV}$	$E_{\text{ads}}(\text{eV})$
1	-57.77	-14.22	-72.40	-0.41
2	-57.77	-14.22	-72.40	-0.41
3	-57.77	-14.22	-72.38	-0.39
4	-57.77	-14.22	-72.38	-0.39
5	-57.77	-14.22	-72.18	-0.19
6	-57.77	-14.22	-72.38	-0.39
7	-57.77	-14.22	-72.38	-0.39
8	-57.77	-14.22	-72.38	-0.39
9	-57.77	-14.22	-72.38	-0.39
10	-57.77	-14.22	-72.33	-0.34
11	-57.77	-14.22	-72.39	-0.40

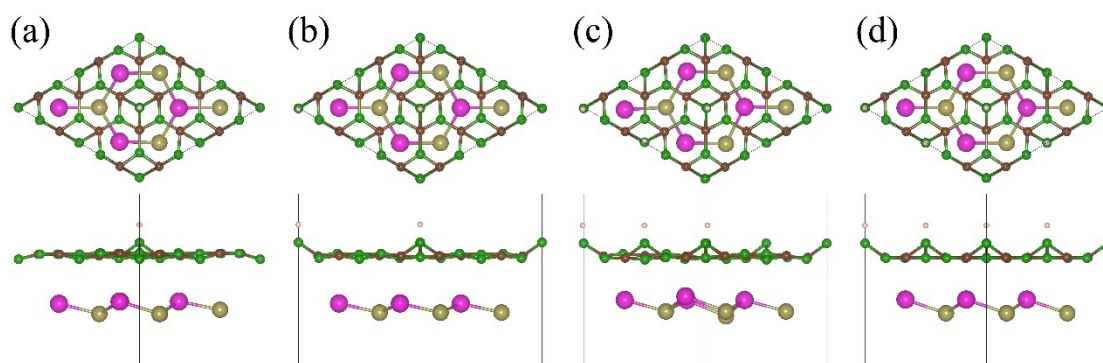


Figure S3 (a), (b), (c) and (d) The optimized structures for different hydrogen coverage on the  $\text{B}_4\text{C}_3$  layer in the  $\text{CdTe}/\text{B}_4\text{C}_3\text{-V}$  heterostructures.

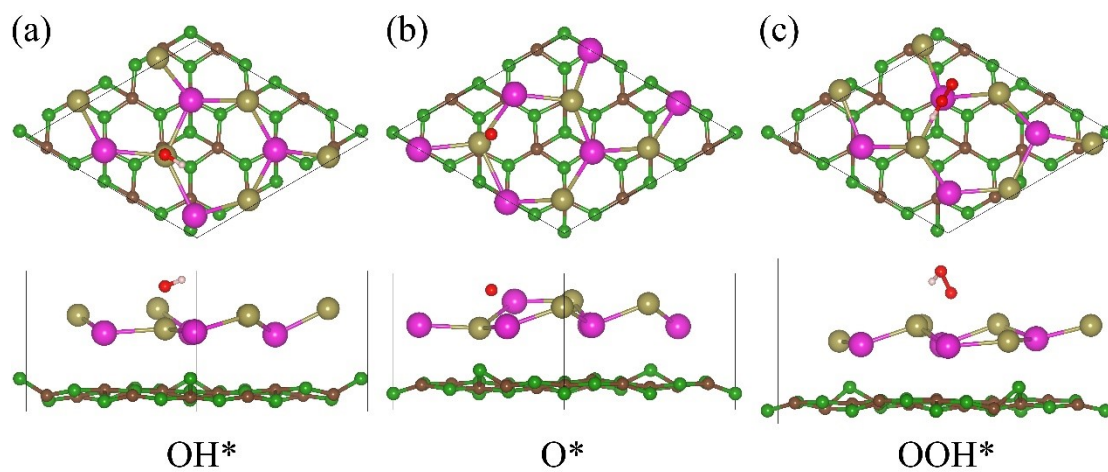


Figure S4 The optimized structures for (a) OH\*, (b) O\* and (c) OOH\* intermediates.