Supporting Information of "Enhanced Photocatalytic Water Splitting with Two-Dimensional van der Waals Heterostructures of BAs/WTeSe"

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AFFILIATIONS

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Phonon spectra calculations

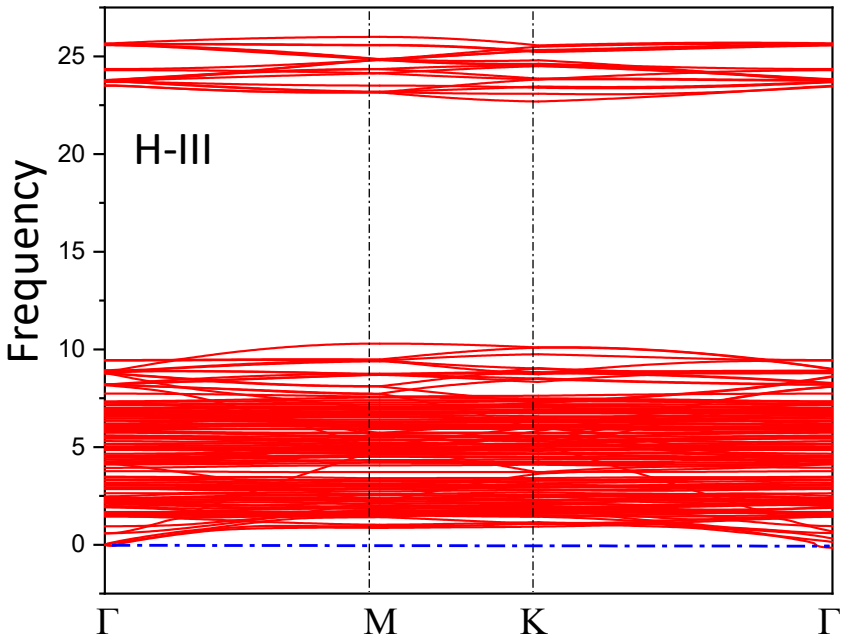

Figure S1. Phonon spectra of the H-III heterostructure.

Ab initio molecular dynamics simulations

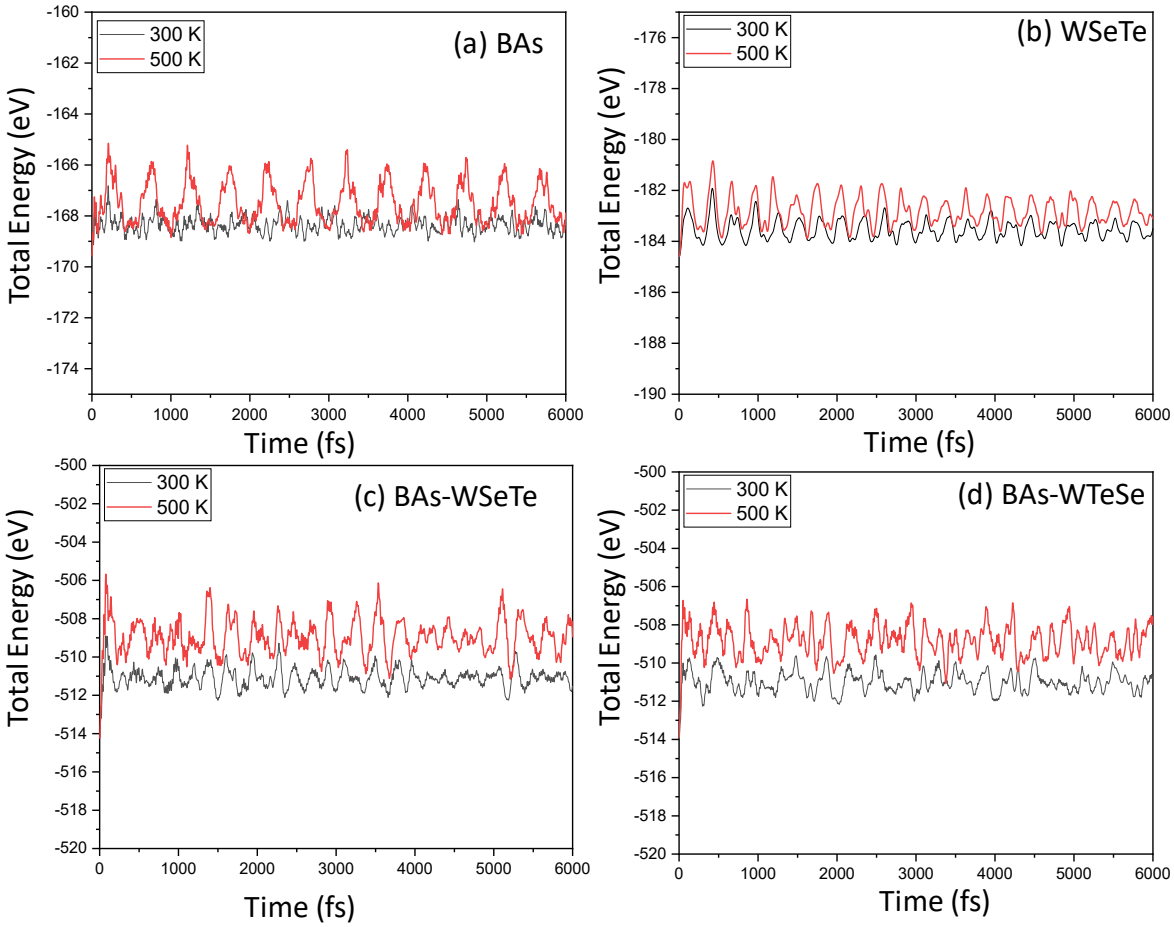

Figure S2. Variation of the total energy of (a) BAs, (b) WSeTe, and (c) BAs-WSeTe and (d) BAs-WTeSe during ab initio molecular dynamics simulations at 300 K and 500 K.

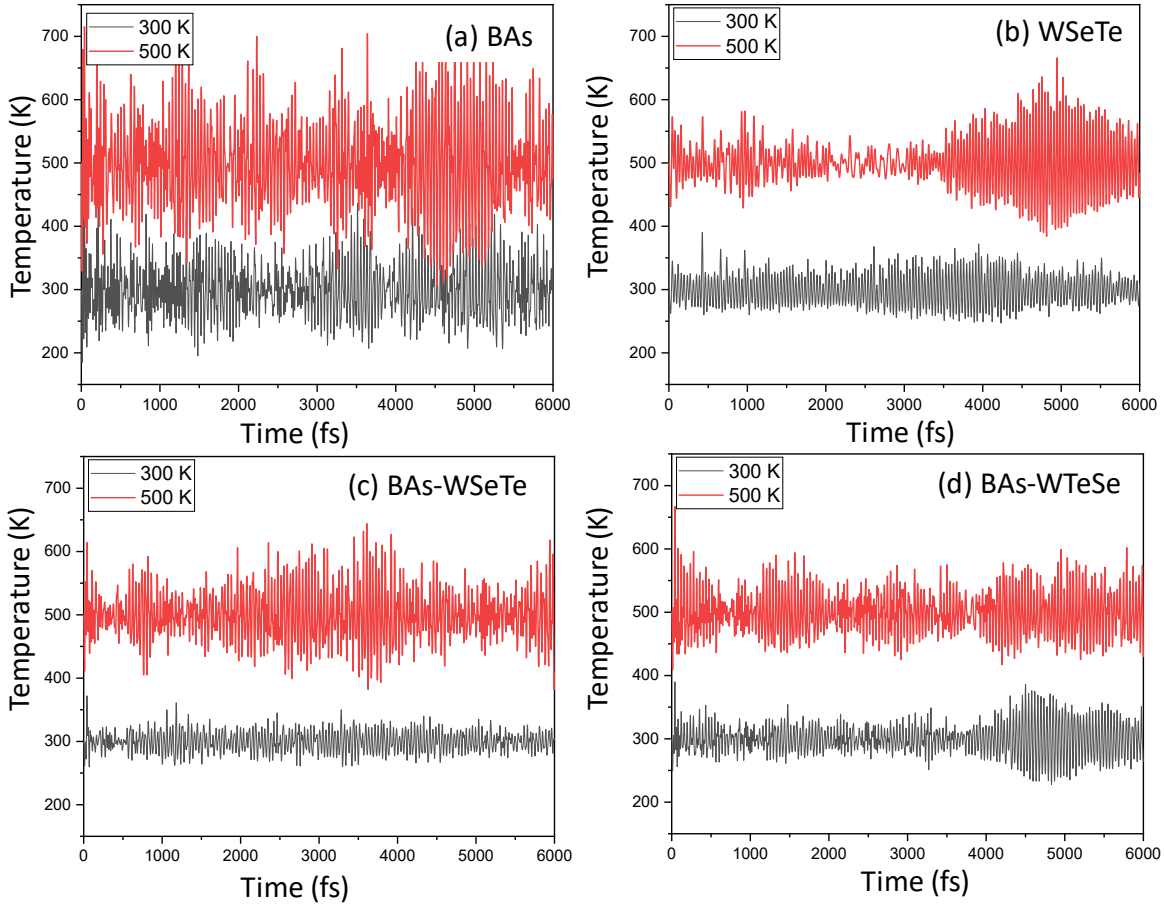

Figure S2A. At 300 K and 500K, the temperature of (a) BAs, (b) WSeTe, and (c) BAs-WSeTe and (d) BAs-WTeSe during the 6 ps ab initio molecular dynamics simulations.

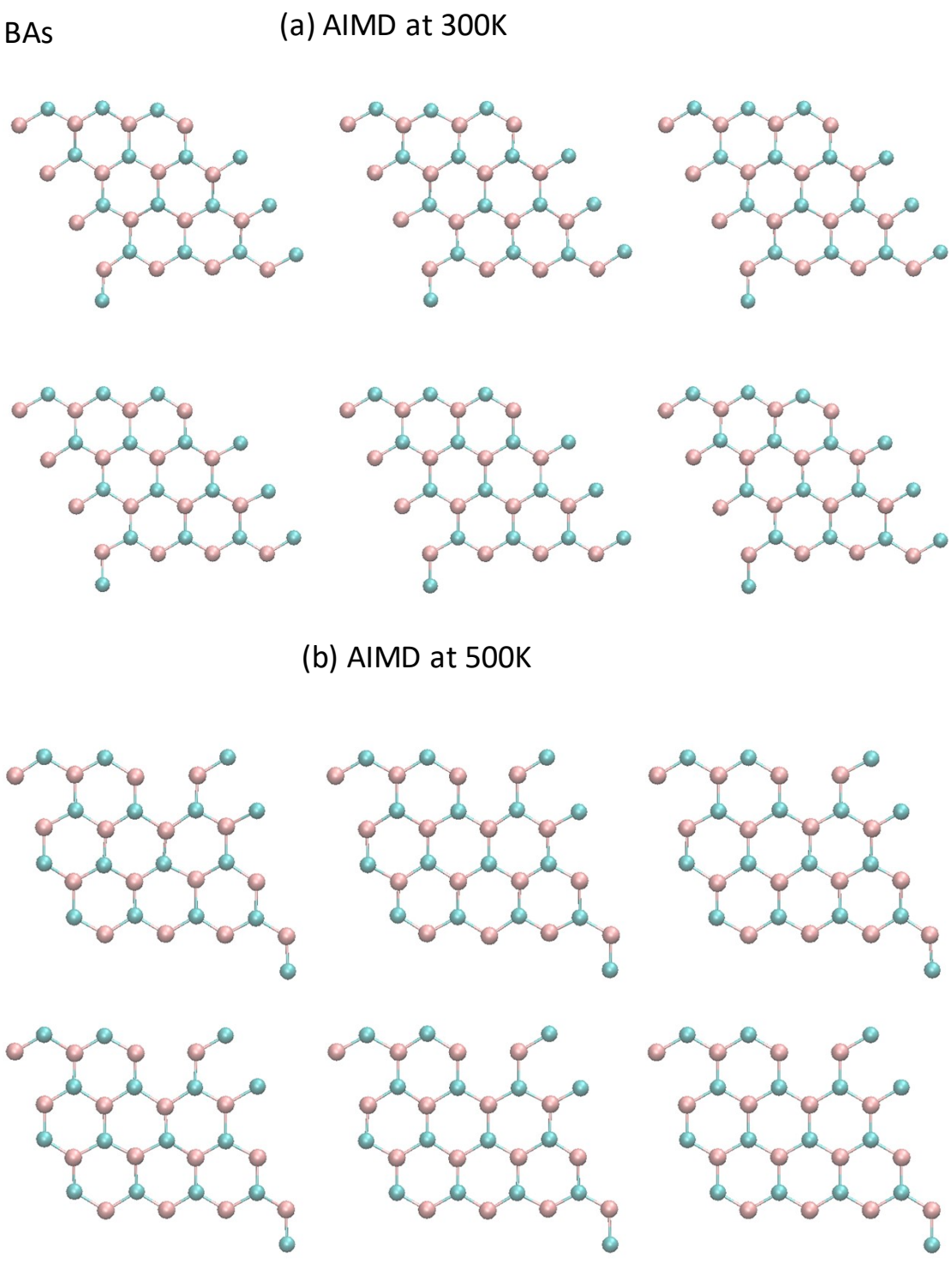

Figure S3. Representative structures of BAs during ab initio molecular dynamics simulations at **(a)** T = 300K and **(b)** T = 500K.

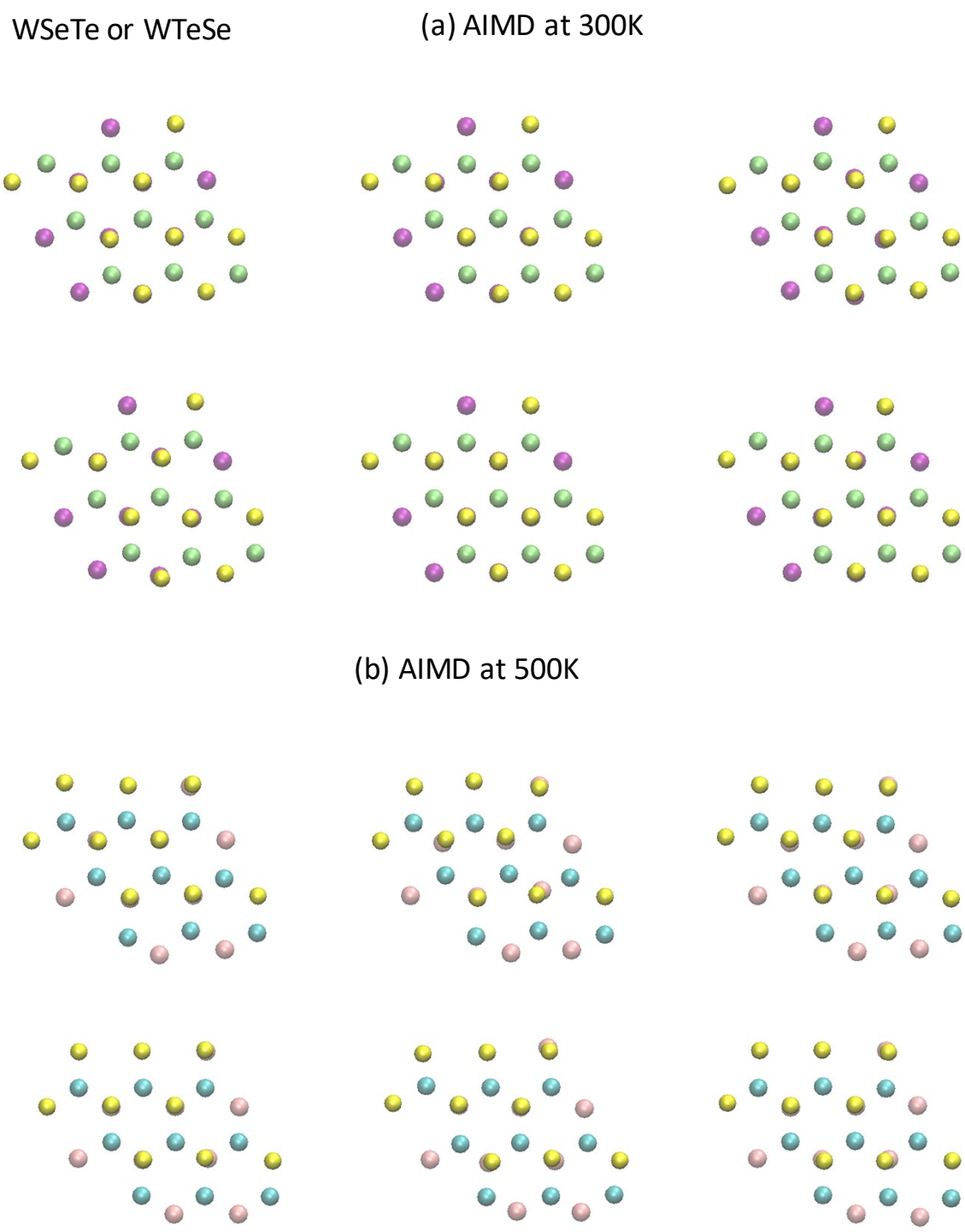

Figure S4. Representative structures of WSeTe during ab initio molecular dynamics simulations at **(a)** T = 300K and **(b)** T = 500K.

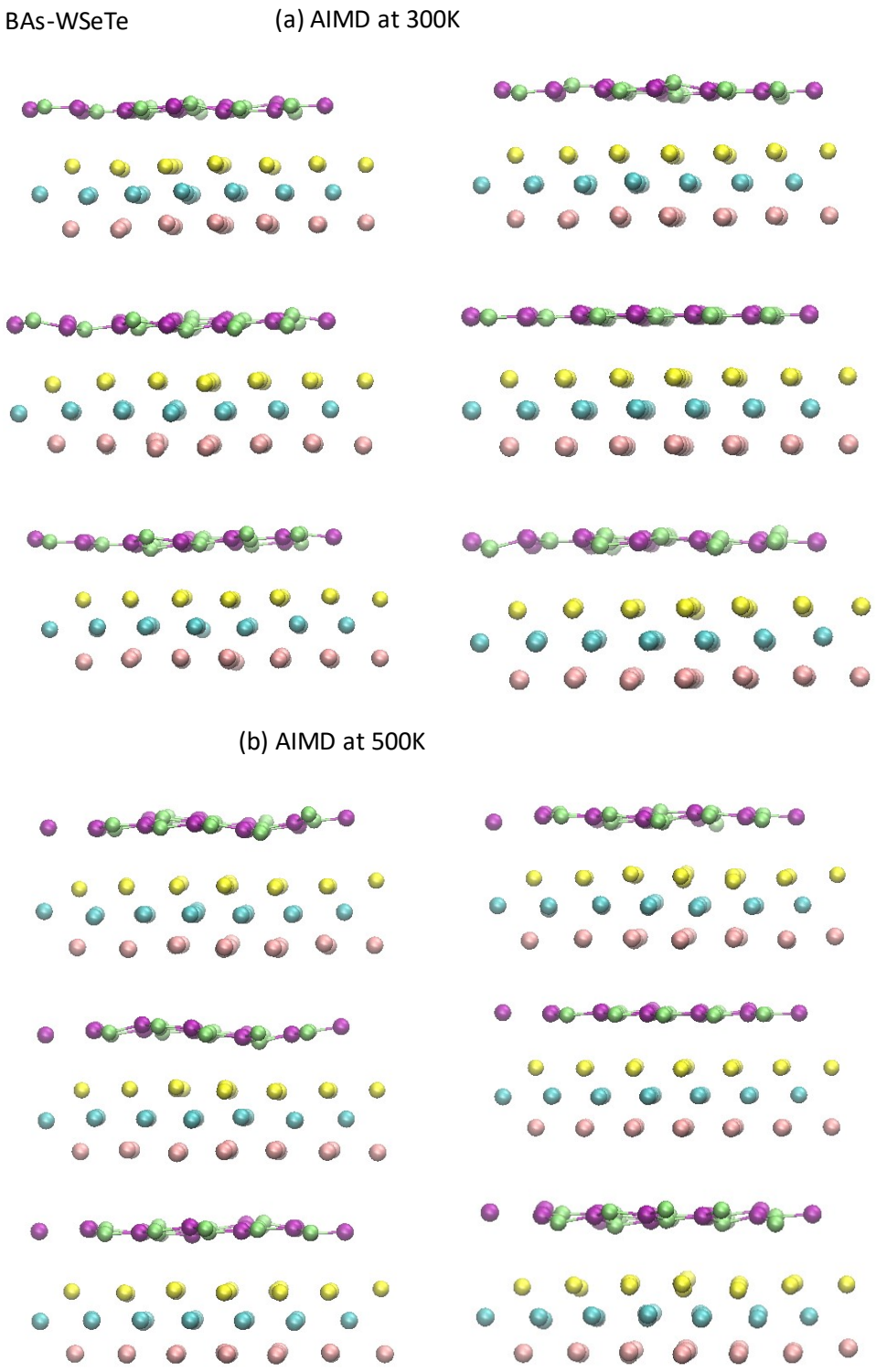

Figure S5. Representative structures of the BAs-WSeTe heterostructure during ab initio molecular dynamics simulations at **(a)** T = 300K and **(b)** T = 500K.

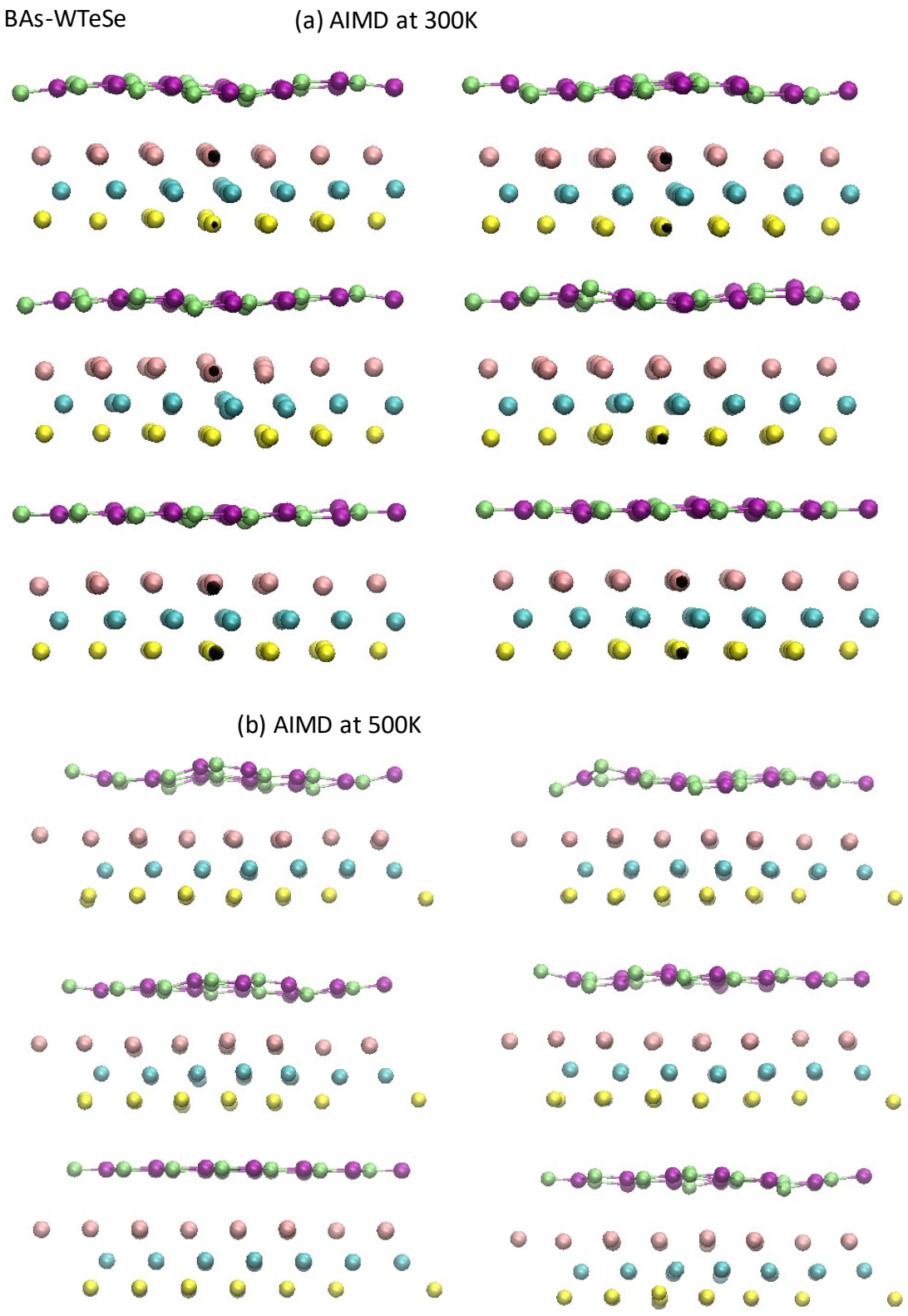

Figure S6. Representative structures of the BAs-WTeSe heterostructure during ab initio molecular dynamics simulations at **(a)** T = 300K and **(b)** T = 500K.

Band structure calculations

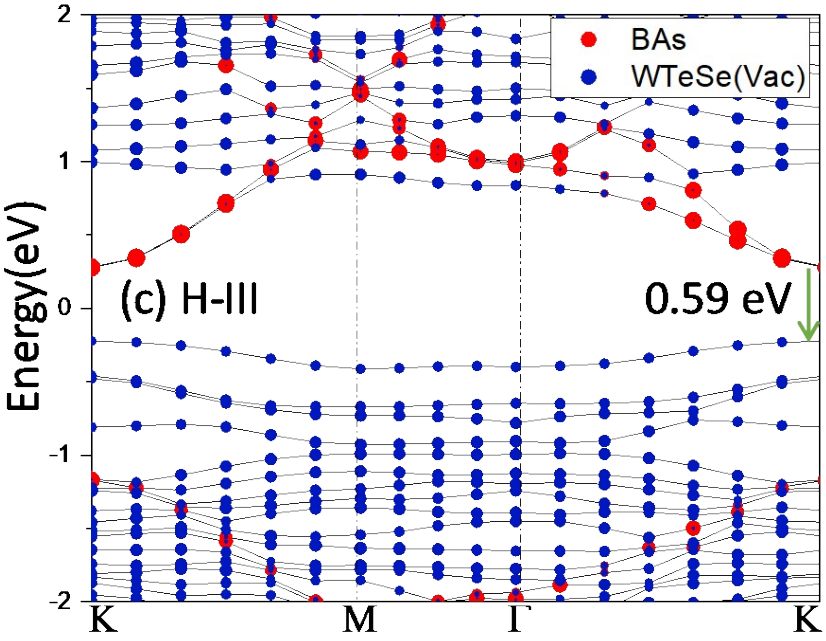

Figure S7. Band structure of the H-III heterostructure.

Photocatalytic water splitting: values of the effective mass

Table S1. Calculated effective mass (m^*) for electrons and holes in the Armchair *x* and zigzag *y* directions (T = 300 K).

	Direction		m^* (m_o)	$D = m^*_h/m^*_e$
BAs	x	Electron	0.173	0.994
		hole	-0.172	
	y	Electron	0.256	0.922
		hole	-0.236	
WSeTe	x	Electron	0.390	1.371
		hole	-0.535	
	y	Electron	0.433	1.559
		hole	-0.675	
H-I	x	Electron	0.184	2.021
		hole	-0.372	
	y	Electron	0.255	1.756
		hole	-0.448	
H-II	x	Electron	0.192	1.875
		hole	-0.360	
	y	Electron	0.277	1.798
		hole	-0.498	
H-III	x	Electron	0.271	0.78
		hole	0.213	
	y	Electron	0.265	2.19
		hole	0.582	
H-IV	x	Electron	0.271	9.11
		hole	2.480	
	y	Electron	0.213	7.55
		hole	1.610	

Calculations of carrier mobilities

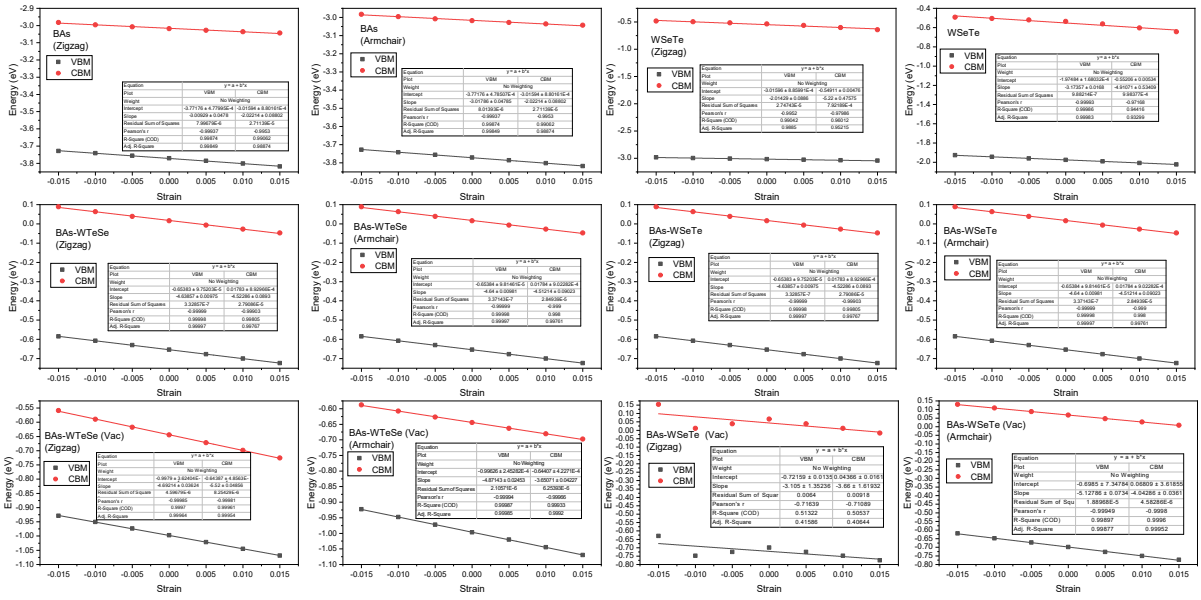

Figure S8. The energy shift of BAs monolayer, WXYsheet, and BAs-Janus WXY(X=Se, Te) obtained from DFT-PBE calculations. Graphs generated using VASPKIT [1].

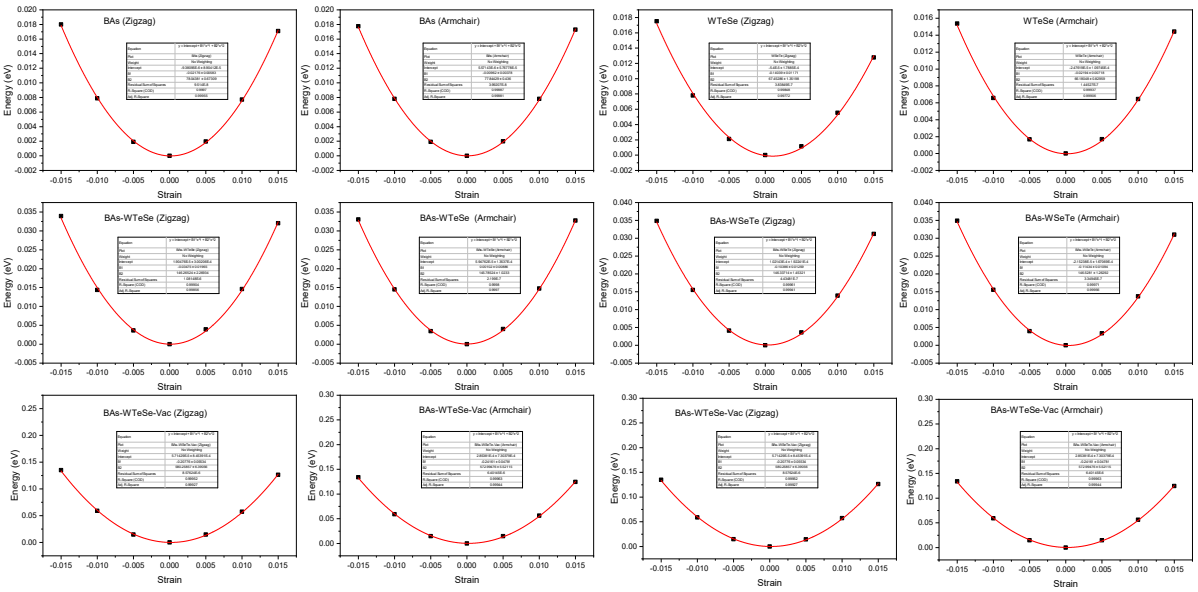

Figure S9. The band edge positions of BAs monolayer, WXY sheet, and BAs-Janus WXY (X=Se, Te) heterostructure as a function of the uniaxial strain obtained from DFT-PBE functional.

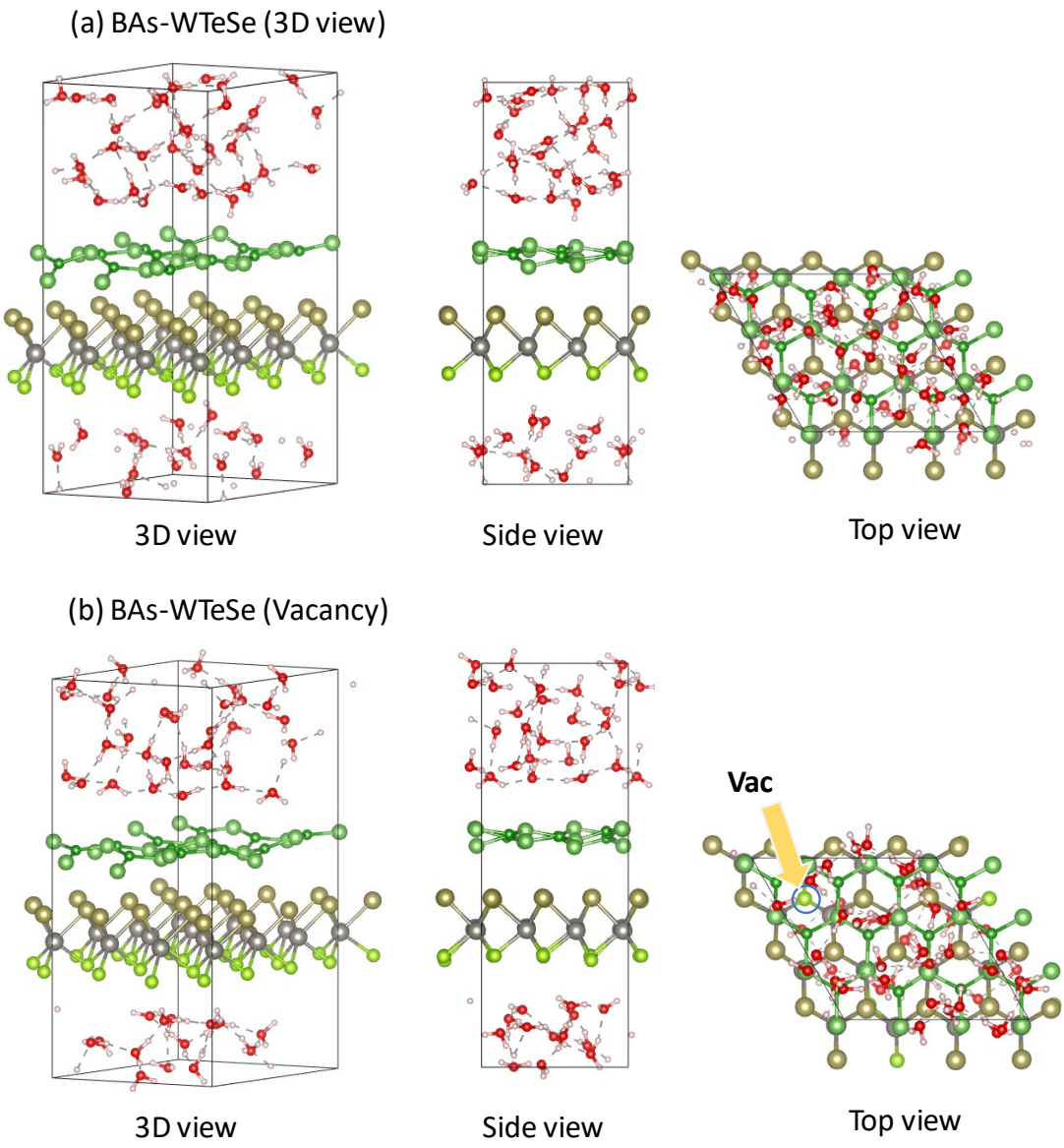

Figure S10. Atomisti model of the heterostructure in contact with water: **(a)** BAs-WTeSe; **(b)** BAs-WTeSe with Te vacancy.

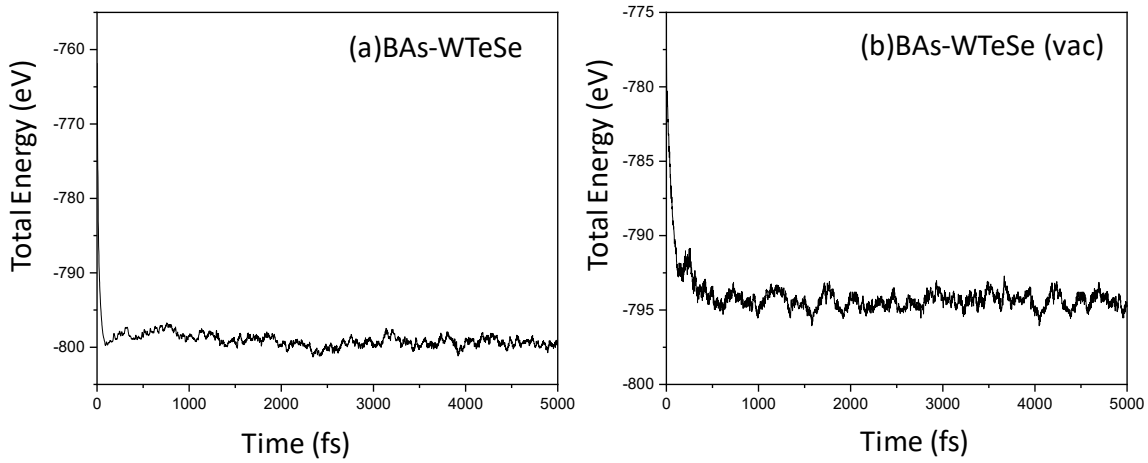

Figure S11. ab initio molecular dynamics simulations for (a) BAs-WTeSe (b) BAs-WTeSe (Vac) at T = 300K

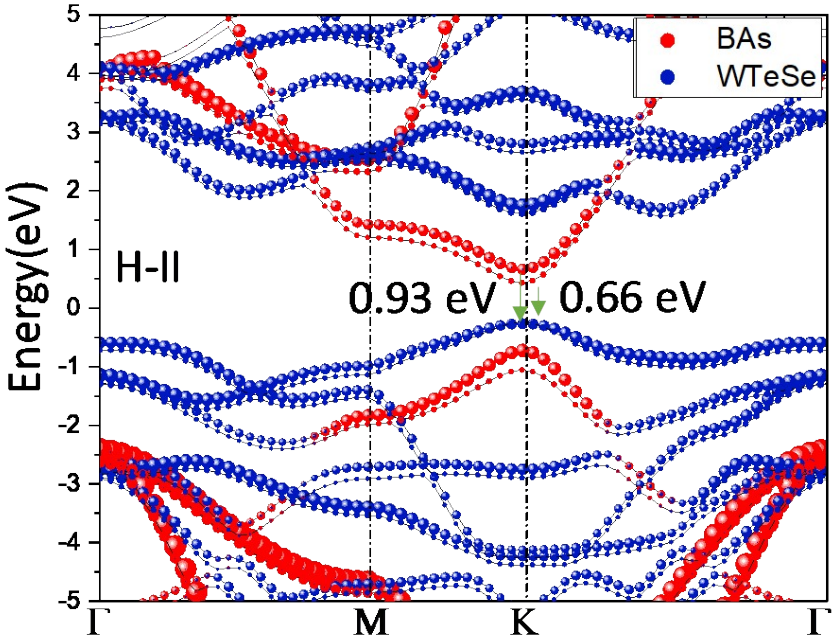

Figure S12 : The band structures with large bubbles for the most stable and small solid circles for the second most stable configuration of WTeSe.

References

[1] V. Wang, N. Xu, J.C. Liu, G. Tang, W.T. Geng, VASPKIT: A User-Friendly Interface Facilitating High-Throughput Computing and Analysis Using VASP Code, Computer Physics Communications 267, 108033 (2021). https://doi.org/10.1016/j.cpc.2021.108033