## **Supporting Information**

## Enhanced photocatalytic activity for water splitting of blue phase

## GeS and GeSe monolayers via biaxial straining

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Figure S1. The phonon spectrum of monolayer GeS and GeSe at (a) (d) -10%, (b) (e) 0% and (c) (f) +10% biaxial strain, respectively.



Figure S2. Band structures (PBE) of monolayer (a) GeS and (b) GeSe.



Figure S3. The partial density of states (HSE06) of monolayer (a)GeS and(b) GeSe.



Figure S4. Band structures (HSE06) of monolayer GeS and GeSe at (a) (e) -10%, (b) (f) -4%, (c)(g) +4% and (d) (h) +10% biaxial strain, respectively.



Figure S5. (a) the Ge-X (X=S, Se) bond length L, the Ge-X (X = S, Se) pucker distance d and (b) the Ge-X (X = S, Se) horizontal angle as a function of biaxial strain of monolayer GeX (X=S, Se).(c) The schematic diagram of monolayer GeX (X=S,



Figure S6. The energy alignment of monolayer GeS at various biaxial strain.



Figure S7. The energy alignment of monolayer GeSe at various biaxial strain.

System	Functional	a(Å)	$d(\text{\AA})$	L(Å)	band gaps	Reference
GeS	LDA	3.383	1.366	2.384	2.446	This work
	Opt88	3.507	1.375	2.447	2.522	This work
	PW91	3.496	1.361	2.435	2.477	This work
	PBE	3.495	1.363	2.435	2.479	This work
	HSE06				3.265	This work
	PBE	3.495	1.363		2.474	[1]
	PBE	3.489	1.36	2.432		[2]
	HSE06				3.27	[2]
GeSe	LDA	3.554	1.451	2.513	2.119	This work
	Opt88	3.685	1.467	2.584	2.291	This work
	PW91	3.676	1.449	2.569	2.274	This work
	PBE	3.676	1.450	2.570	2.276	This work
	HSE06				2.993	This work
	PBE	3.674	1.451		2.274	[1]
	PBE	3.663	1.45	2.566		[2]
	HSE06				3.01	[2]

Table S1. The lattice constants a (Å), sheet thickness d (Å), the Ge-X (X = S, Se) bond length L (Å) and band gaps (eV) of monolayer GeX (X = S, Se)

## Reference

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- 2. Ji, Y.; Yang, M.; Dong, H.; Hou, T.; Wang, L.; Li, Y. *Nanoscale* 2017, **9**, (25), 8608-8615.