

**A Density functional theory study on the strain modulated electronic and photocatalytic properties of GaSe monolayer for photocatalytic water splitting and artificial photosynthesis**

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Table S1. The reported summary of the calculated lattice constant and band gap values of the GaSe monolayer using different types vdW interactions.

Sl. No.	Lattice constant(Å)	Bandgap (eV)		Types of structure studied	Bandgap tuning	Applications	References
		PBE	HSE				
1.	3.82	1.83	2.71	Monolayer	Strain	Device modeling	[1]
2.	3.84	1.82	2.9	Heterostructure	Strain, electric field	Optoelectronic nanodevices	[2]
3.	-	2.23	-	Heterostructure	-	Optoelectronic	[3]
4.	3.82	1.91	2.98	Monolayer	Strain	Water splitting	[4]
5.	3.78	1.6	-	Heterostructure	Strain, electric field	Nanoelectronics devices	[5]
6.	3.82	-	2.69	Monolayer	-	Transistors	[6]
7.	3.82	2.1	-	Monolayer	-	Thermoelectric	[7]
8.	3.75	2.21	-	Monolayer	Strain	Electromechanical	[8]
9.	3.75	2.23	-	Monolayer	Doping	-	[9]
10.	3.82	1.78	2.64	Heterostructure	-	Solar energy Harvesting	[10]
11.	3.82	1.77	2.93	Monolayer	Strain	water splitting and artificial photosynthesis	This work

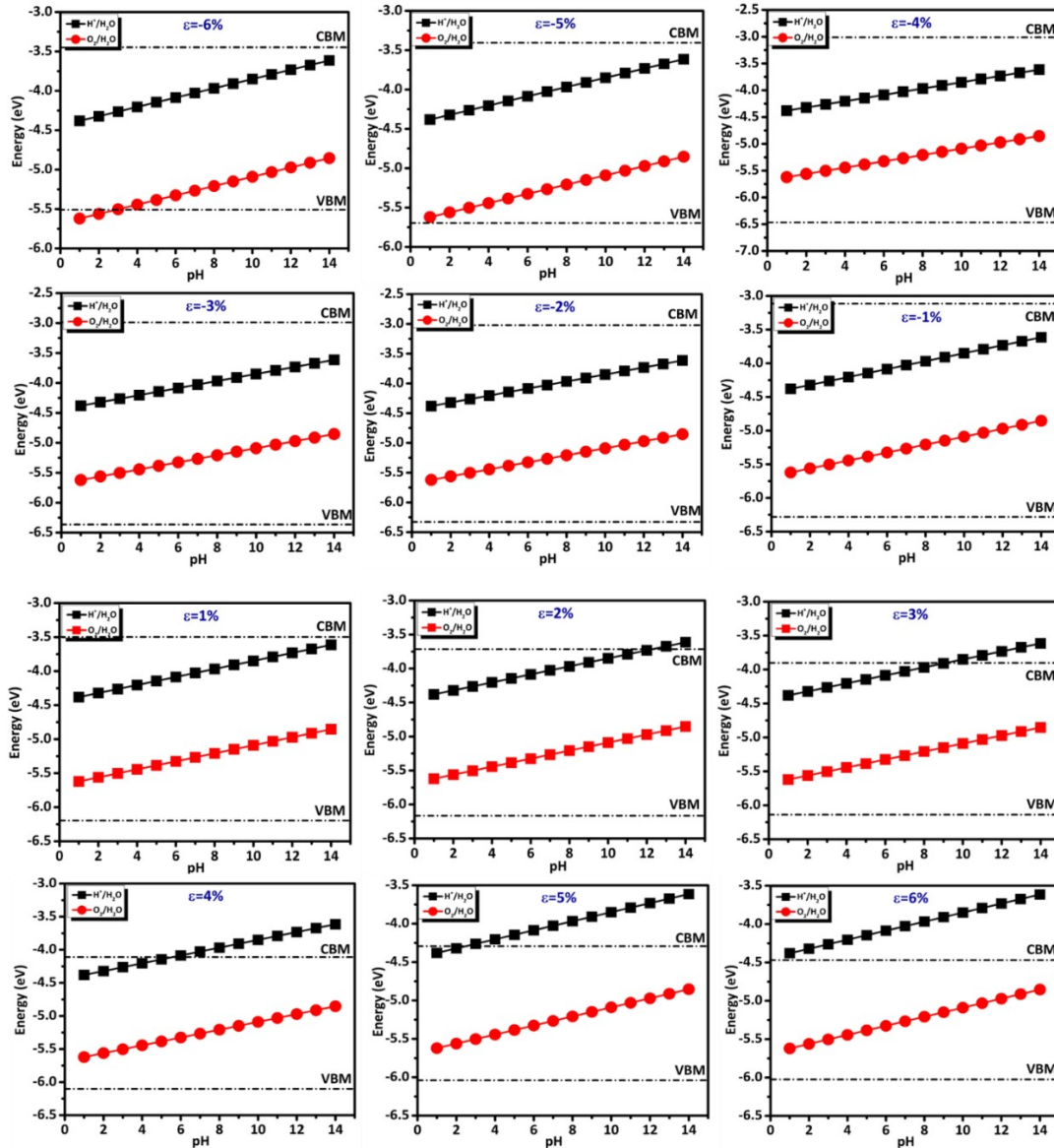


Figure S1. The effect of pH on the water redox potentials for water splitting.

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