Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Enhanced photocatalytic properties of a chemically modified blue phosphorene

Ashakiran Maibam,[a,b#]*Sawan Kumar Das,*[a#] *,Pragnya paramita Samal* [a,b] *Sailaja Krishnamurty**[a,b]

[a]Physical and Materials Chemistry Division,

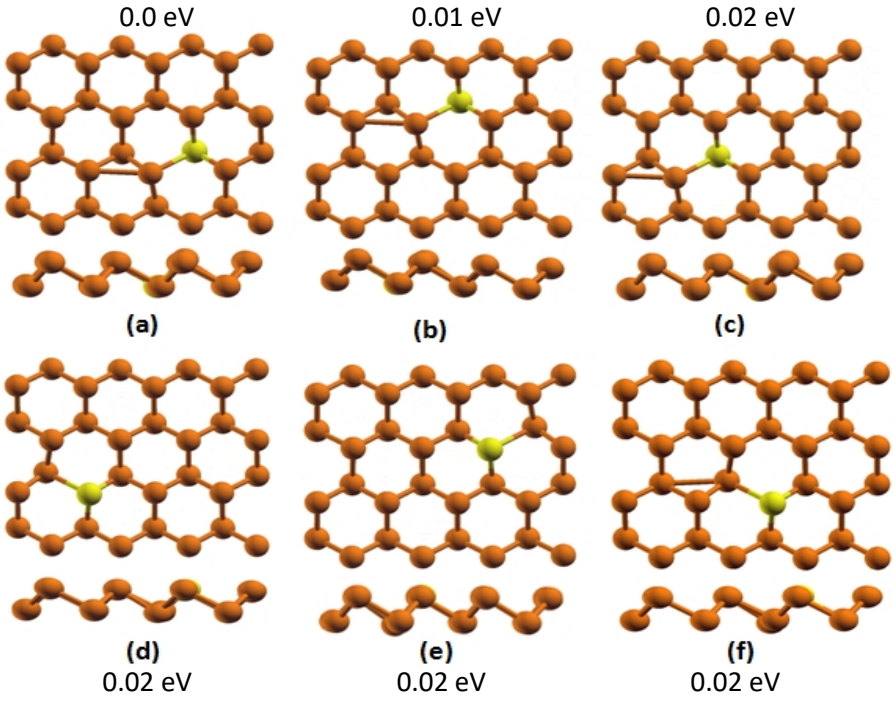
National Chemical Laboratory, Pashan Road, Pune 411008, India

[b]Academy of Scientific and Innovative Research, CSIR-Human Resource Development Centre (CSIR-HRDC) Campus, Postal Staff College area, Gaziabad, 201 002 Uttar Pradesh, India

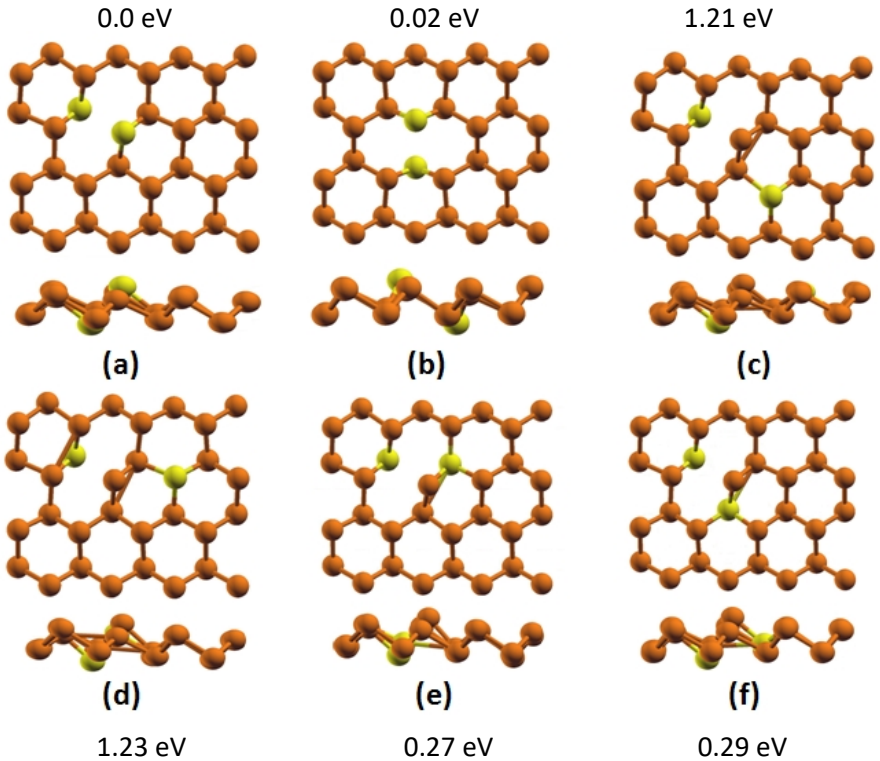
e-mail: k.sailaja@ncl.res.in, sailaja.raaj@gmail.com

Contents:

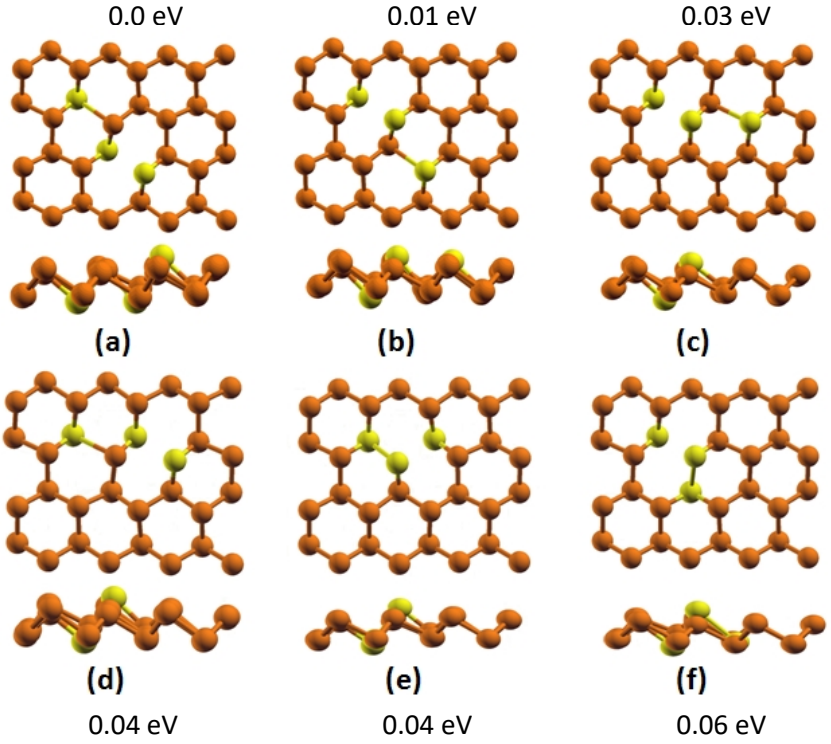
# Equal contribution to the work



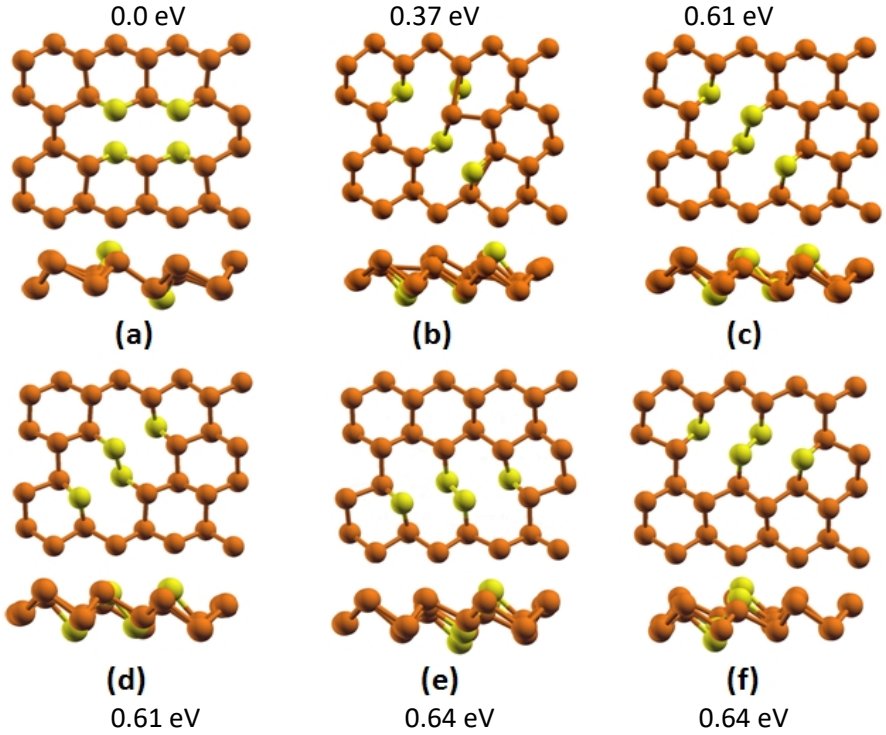
S.F.1: Six lowest energy conformations of 1S-B-phosphorene and relative energies are given in eV in top and bottom.



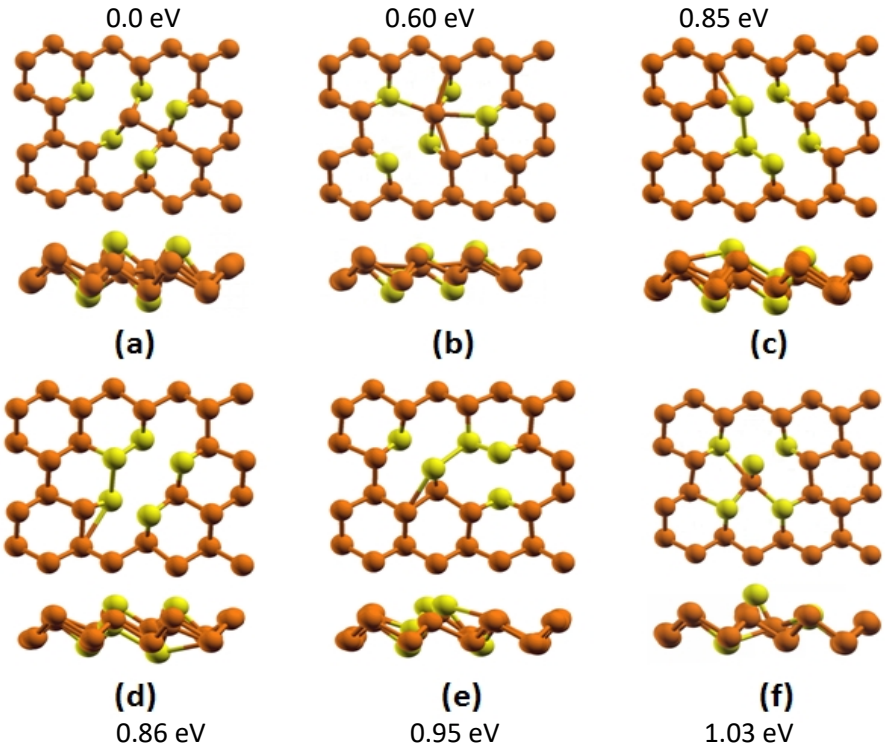
S.F.2: Six lowest energy conformations of 2S-B-phosphorene and relative energies are given in eV in top and bottom.



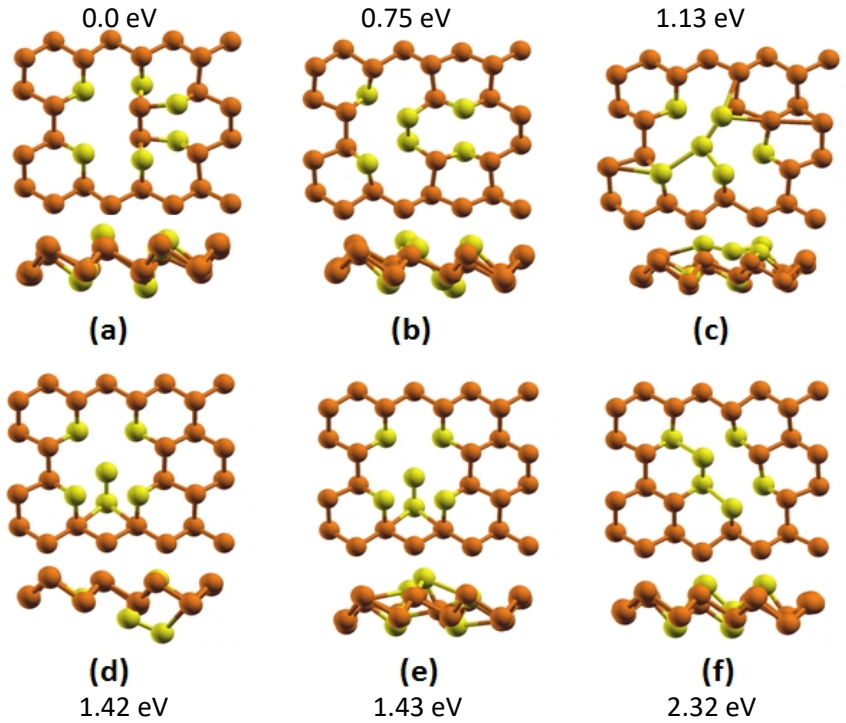
S.F.3: Six lowest energy conformations of 3S-B-phosphorene and relative energies are given in eV in top and bottom.



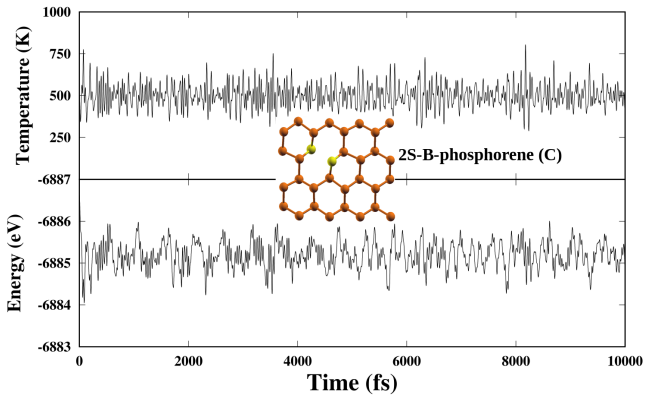
S.F.4: Six lowest energy conformations of 4S-B-phosphorene and relative energies are given in eV in top and bottom.



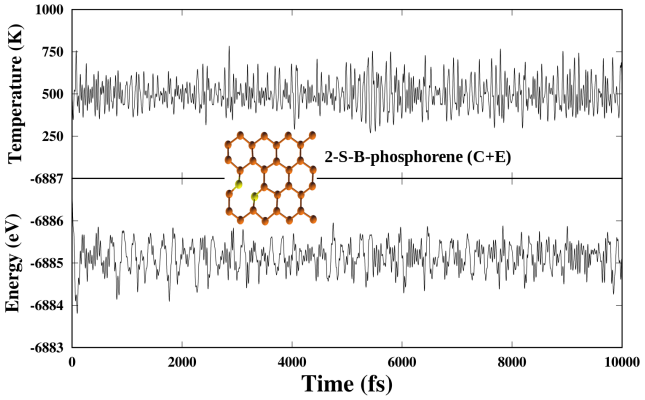
S.F.5: Six lowest energy conformations of 5S-B-phosphorene and relative energies are given in eV in top and bottom.



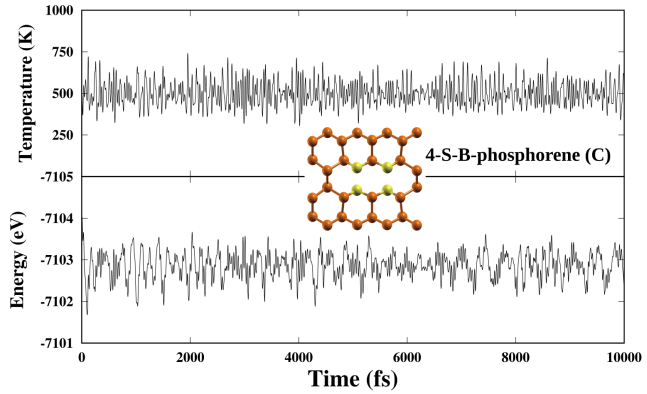
S.F.6: Six lowest energy conformations of 6S-B-phosphorene and relative energies are given in eV in top and bottom.



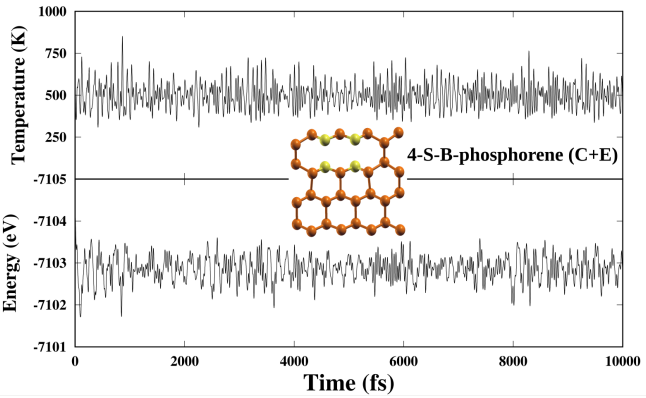
(a) 2-S-B-phosphorene(C) AIMD plot at 500K for 10 ps.



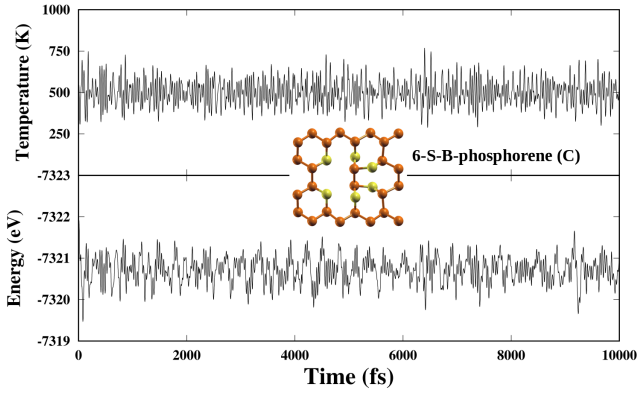
(b) 2-S-B-phosphorene(C+E) AIMD plot at 500K for 10 ps.



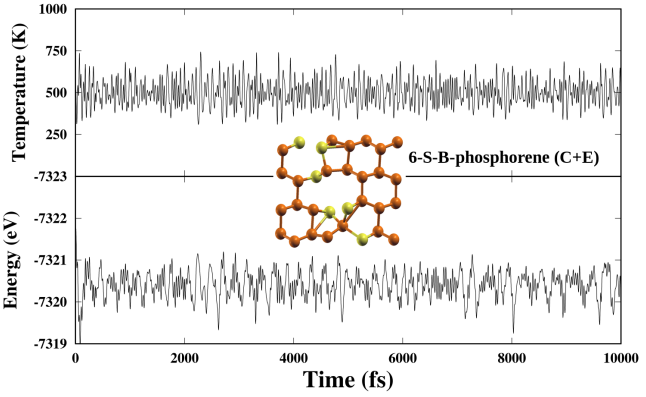
(c) 4-S-B-phosphorene(C) AIMD plot at 500K for 10 ps.



(d) 4-S-B-phosphorene(C+E) AIMD plot at 500K for 10 ps.



(e) 6-S-B-phosphorene(C) AIMD plot at 500K for 10 ps.



(f) 6-S-B-phosphorene(C+E) AIMD plot at 500K for 10 ps.

S.F.7: AIMD plots of 2S-B-phosphorene, 4S-B-phosphorene and 6S-B-phosphorene with sulphur dopants at C and C+E sites at 500K.

*n*B-phosphorene		E_{ad} (eV)	O-H Bondlength (Å)	O-H-O angle (°)	S-H bond distance (Å)	E_g (eV)	Symmetric frequency of OH_1 (cm^{-1})	Asymmetric frequency of OH_2 (cm^{-1})	Redshift in Symmetric frequency (cm^{-1})
2	C	-0.50	0.976, 0.976	104.3	2.45	1.91	3503.8	3647.2	203.8
	E	-0.59	0.982, 0.971	106.4	2.81	1.91	3436.9	3695.2	270.6
	C+E	-0.58	0.981, 0.970	106.4	2.88	1.92	3444.9	3702.8	262.6
	C+E	-0.51	0.980, 0.972	104.6	3.05		3448.6	3684.0	259
4	C	-0.52	0.974, 0.974	104.0	2.42	1.71	3525.7	3659.1	181.8
	E	-0.59	0.981, 0.980	103.8	2.25	1.82	3430.3	3553.1	277.3
	C+E	-0.53	0.974, 0.974	104.2	2.43	1.75	3529.6	3669.7	178
	C+E	-0.54	0.978, 0.972	104.3	2.31		3497.7	3694.7	209.9
6	C	-0.59	0.980, 0.973	105.3	2.27	1.58	3468.4	3681.4	239.2
	E	-0.55	0.981, 0.971	105.5	2.80	1.74	3442.6	3692.9	265
	C+E	-0.65	0.984, 0.975	104.4	2.24	1.75	3410.8	3615.0	296.8
	C+E	-0.61	0.979, 0.973	104.9	2.58		3488.7	3677.7	218.9
B-phosphorene		-0.43	0.976, 0.975	103.7	2.40	2.00	3504.2	3628.4	203.4

S.T.1: Table detailing various parameters for water activation.

Where $\mathbf{E_{ad}}$ is the adsorption energy of water on PNS (Phosphorene Nanosheet) $\mathbf{E_g}$ is the bandgap of B-PNS without water, C- centre, E- Edge. The highlighted and red coloured letter in C+E corresponds to the site on which water molecule is adsorbed.