Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Electronic Supplementary Information

Blue phosphorene/Sc_2CX_2 (X = O, F) van der Waals Heterostructures as suitable candidates for water-splitting photocatalysts and solar cells

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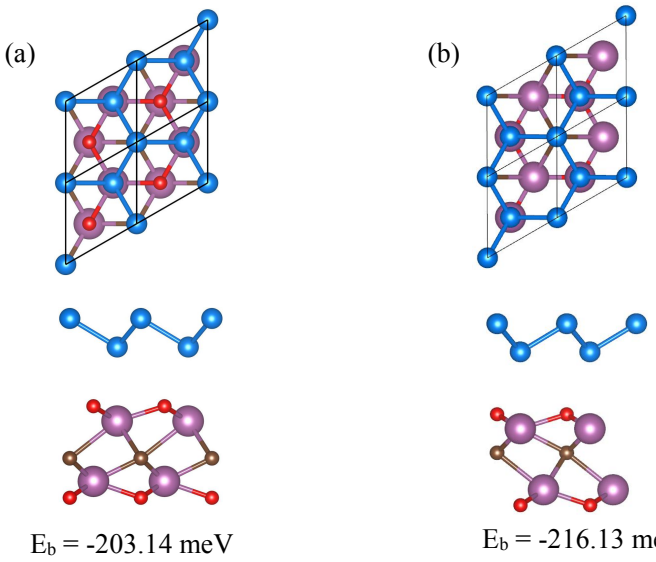

Fig**. S1.** Top and side views of (a) α-type and (b) β-type BlueP/Sc_2CO_2 heterostructures.

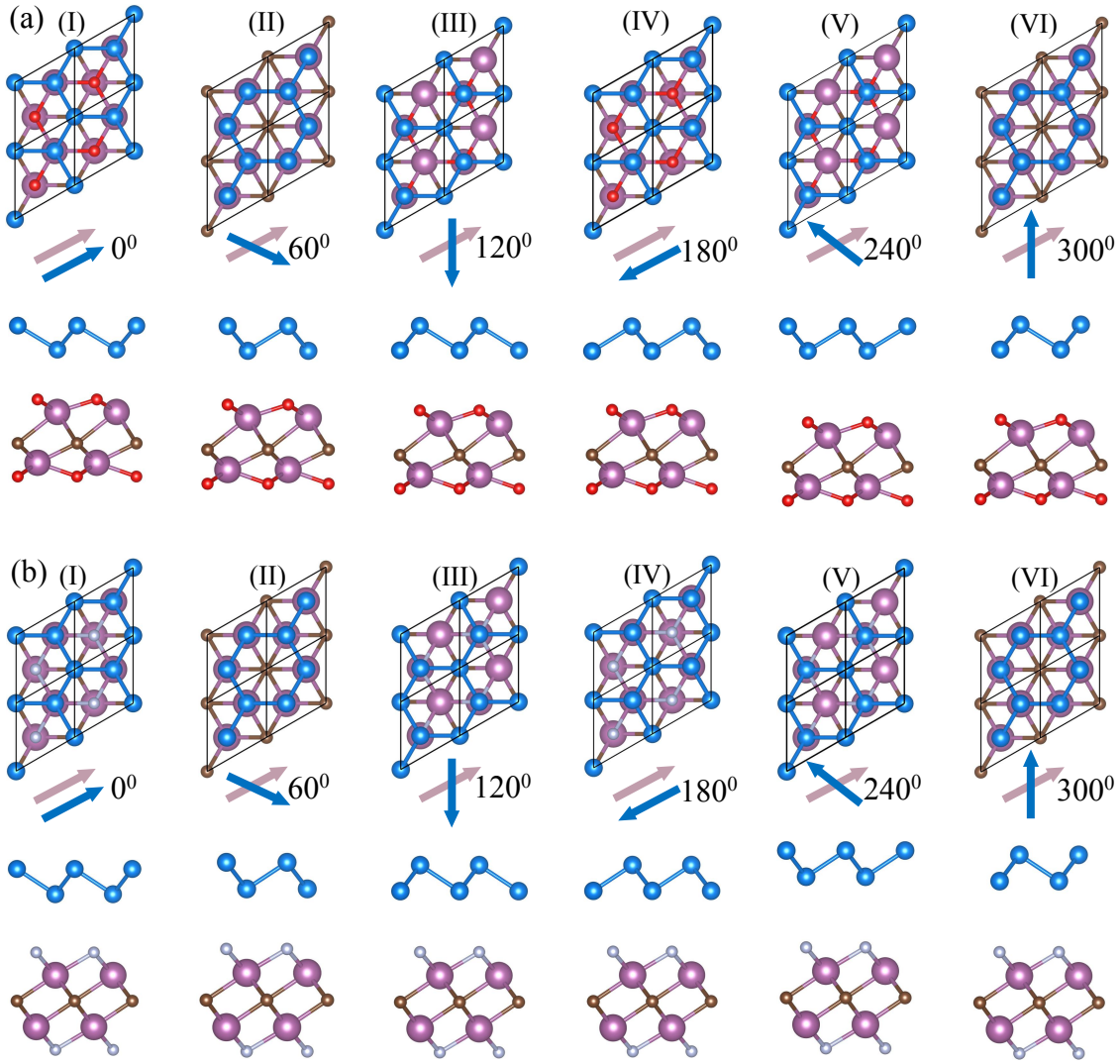

FIg. **S2**. Top and side views of (a) BlueP/Sc_2CO_2 and (b) BlueP/Sc_2CF_2 heterostructures with different stacking confifigurations in terms of rotation 60^0 angles of the BlueP monolayer with respect to Sc_2CX_2 .

Table **S1**. Binding energy per unit cell (E_b/meV) and the interlayer distance (D/Å) of BlueP/Sc_2CX_2 heterostructures for six confifigurations (I-VI). The bold values represent the largest binding energy among different stackings.

Congfiguration	I		II		III		IV		V		VI	
	E_b	D	E_b	D	E_b	D	E_b	D	E_b	D	E_b	D
BlueP/Sc_2CO_2	**-203.24**	2.48	-198.88	2.61	-148.76	2.97	-153.41	2.88	-71.37	3.54	-75.04	3.41
BlueP/Sc_2CF_2	-142.40	2.85	**-143.74**	2.80	-132.51	2.90	-130.61	2.91	-78.75	3.34	-78.43	3.35

Table **S2**: Macroscopic static dielectric constants (ε), effective mass (m/m_0), and exciton binding energies (E_{eb}/eV) of BlueP/Sc_2CX_2 heterostructures

	ε_{ion}			ε_{el}			m_e	m_h	E_{eb}
	x	y	z	x	y	z			
BlueP	0	0	0	2.19	2.19	1.10	0.67	1.13	1.19
Sc_2CO_2	2.55	2.55	0.08	2.91	2.91	1.32	1.06	1.06	0.24
Sc_2CF_2	8.86	8.87	0.08	3.89	3.89	1.32	0.61	2.19	0.04
BlueP/Sc_2CO_2	1.22	1.22	0.03	3.11	3.11	1.27	0.19	0.98	0.12
BlueP/Sc_2CF_2	4.39	4.37	0.04	3.62	3.62	1.27	0.79	0.54	0.07

Discussion S1:

In the Scharber's formalism for calculating PCE, the gap of donor material is the optical gap, which is usually less than the electronic gap. In fact, the electronic gap calculated with HSE method is less than experimental electronic band gap. So far, there is no experimental optical band gap available for BlueP and Sc_2CX_2. In the case of phosphorene, HSE06 gives a result of 1.49 eV, which is very close to the optical band gap (1.45 eV) [1]. Similar results also exist for MoS_2 monolayer [1]. This good agreement between the HSE06 band gaps and experimental optical band gaps is, of course, by coincidence and has no real physics. Therefore, in our work, it should be reasonable to take the HSE06 band gap to represent the gaps of donor materials for calculating the power conversion efficiency.

References

[1] Li, Y. G.; Li, Y. L.; Sa, B. S.; Ahujad, R. Review of Two-Dimensional Materials for Photocatalytic Water Splitting from a Theoretical Perspective. *Catal. Sci. Technol.* **2017**, 7, 545–559.