Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Phase-dependant electrocatalytic activity of colloidally synthesized WP and α-WP_2 electrocatalysts for hydrogen evolution reaction

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ADDITIONAL SUPPORTING INFORMATION

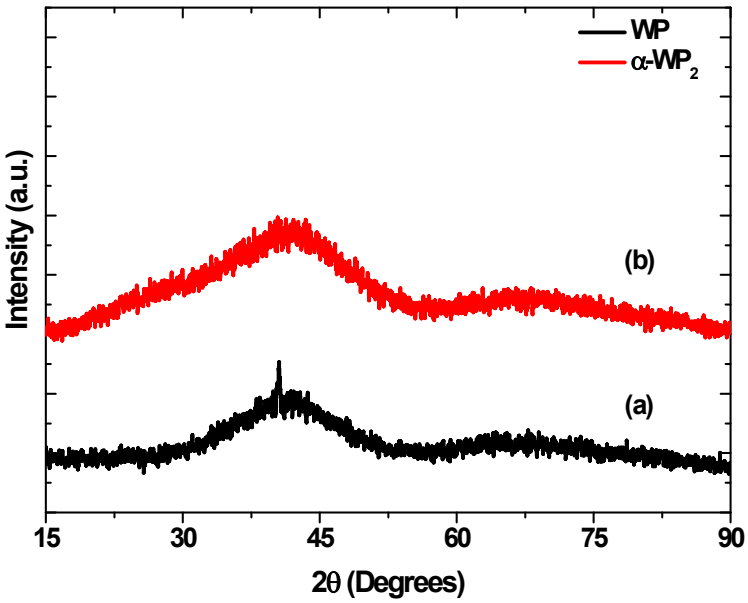


Figure S1: X-ray diffraction pattern of as synthesized (a) WP and (b) α-WP_2.

Calculations of the interplanar spacing from the XRD results:

WP (011)

2θ = 31.115

θ = 15.5575, λ = 0.15460 nm

λ = 2dSinθ

d = 0.15406 nm/2Sinθ = 0.2871 nm

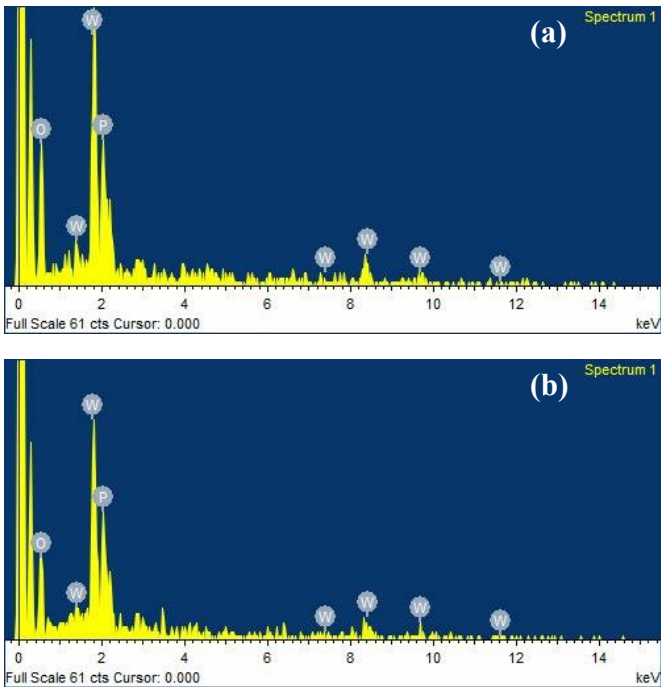
A-WP_2 (-201)

2θ = 20.971

θ = 10.4855, λ = 0.15460 nm

λ = 2dSinθ

d = 0.15406 nm/2Sinθ = 0.4231 nm



Element	Atomic %
O	76.82
P	12.39
W	10.79

Element	Atomic %
O	70.86
P	17.36
W	11.78

Figure S2: EDX spectra and corresponding atomic % of (a) WP and (b) α-WP_2.

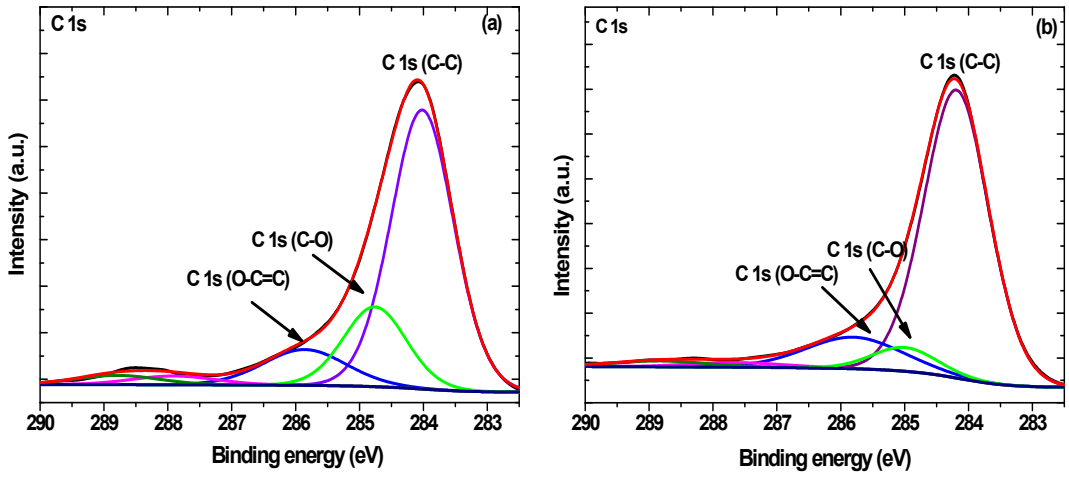


Figure S3: The C 1s spectrum of (a) WP and (b) α-WP_2.

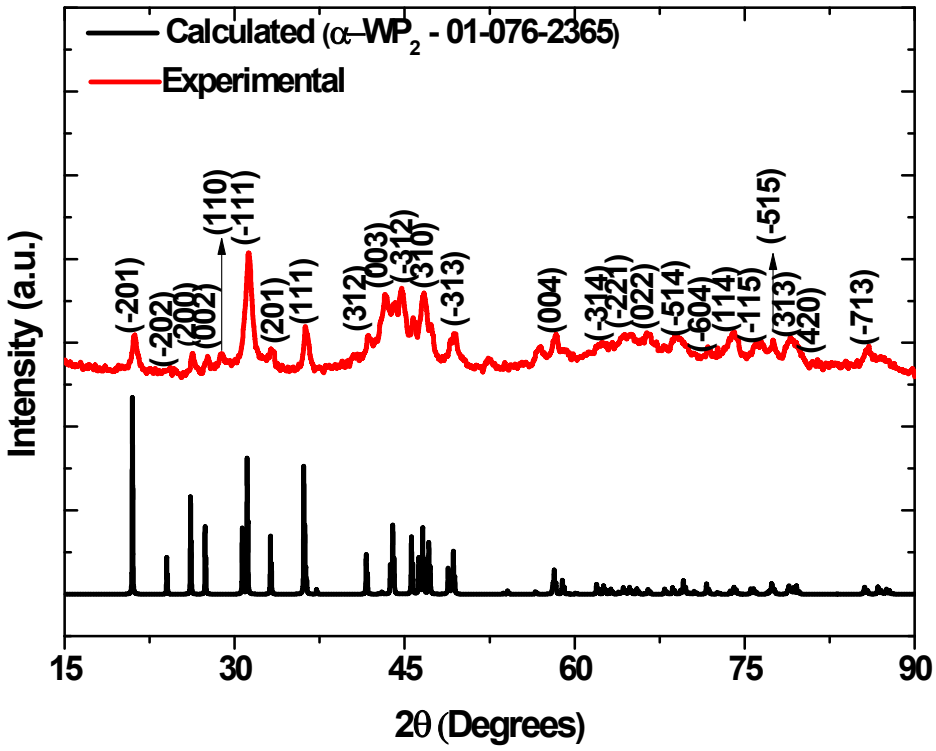


Figure S4: XRD pattern of long term stored α-WP_2.

Table S1: : Comparison of the electrocatalytic activity of WP and α-WP_2 catalysts

Catalyst	Tafel Slope (mV dec^{-1})	Overpotential (10 mA cm^{-2})	Exchange current density (mA cm^{-2})	Onset potential (mV)
WP	95.71	314	0.004239	145
α-WP_2	86.83	271	0.004536	106

Table S2: Kinetic parameters of WP and α-WP_2 catalysts

Catalyst	T(K)	β (mV/dec)	J_0 ($mAcm^{-2}$)	E_a (kJ/mol)
WP	298	95.71	0.004239	44.24
	308	92.58	0.006973	
	318	87.34	0.0.01136	
	328	84.59	0.01316	
α-WP_2	298	86.83	0.004536	31.79
	308	84.86	0.009468	
	318	82.72	0.01023	
	328	80.25	0.02410	

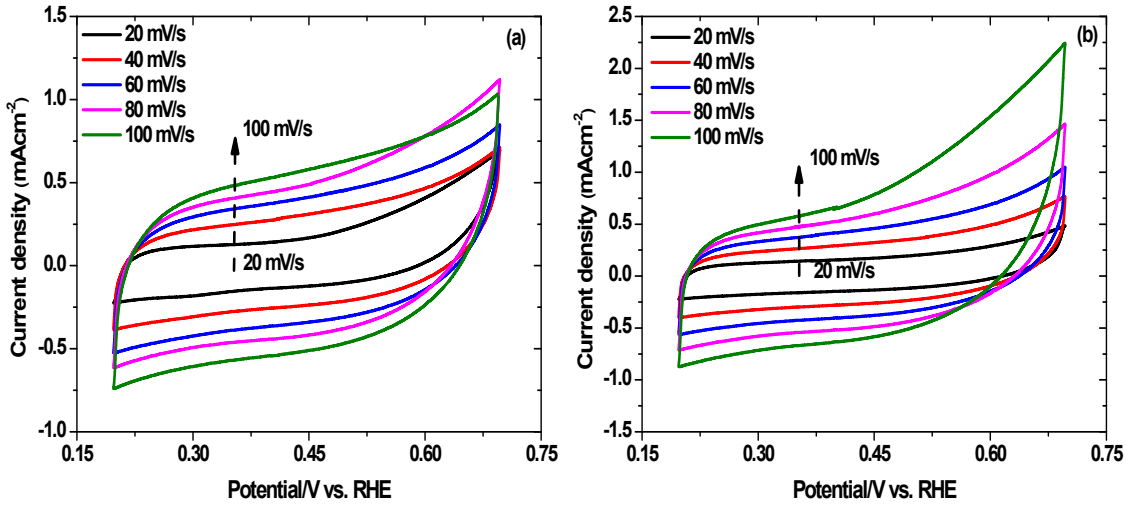


Figure S5: Cyclic Voltammetry (CV) curves of (a) WP and (b) α-WP_2 catalysts measured in a potential window without faradaic processes in 0.5 M H_2SO_4 at scan rate from 20 - 100 mV s^{-1}.

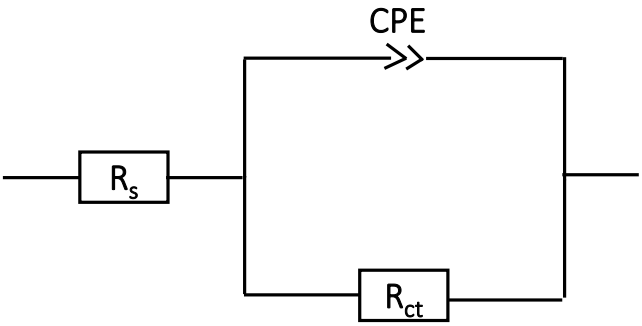


Figure S6: Equivalent circuit for one time constant, where R_s - solution resistant; CPE - constant phase element; R_{ct} – charge transfer resistance.

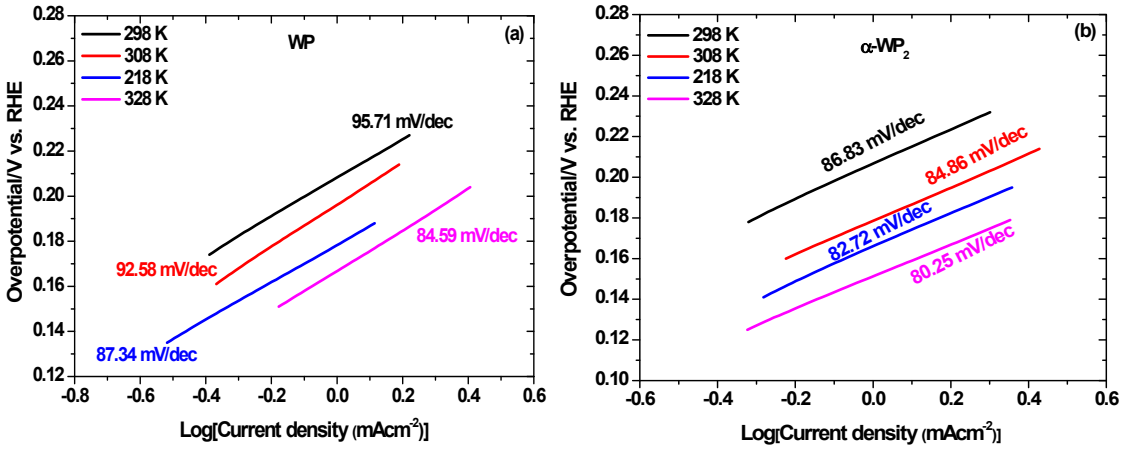


Figure S7: Tafel slopes of (a) WP and (b) α-WP_2 catalysts obtained at different temperatures.

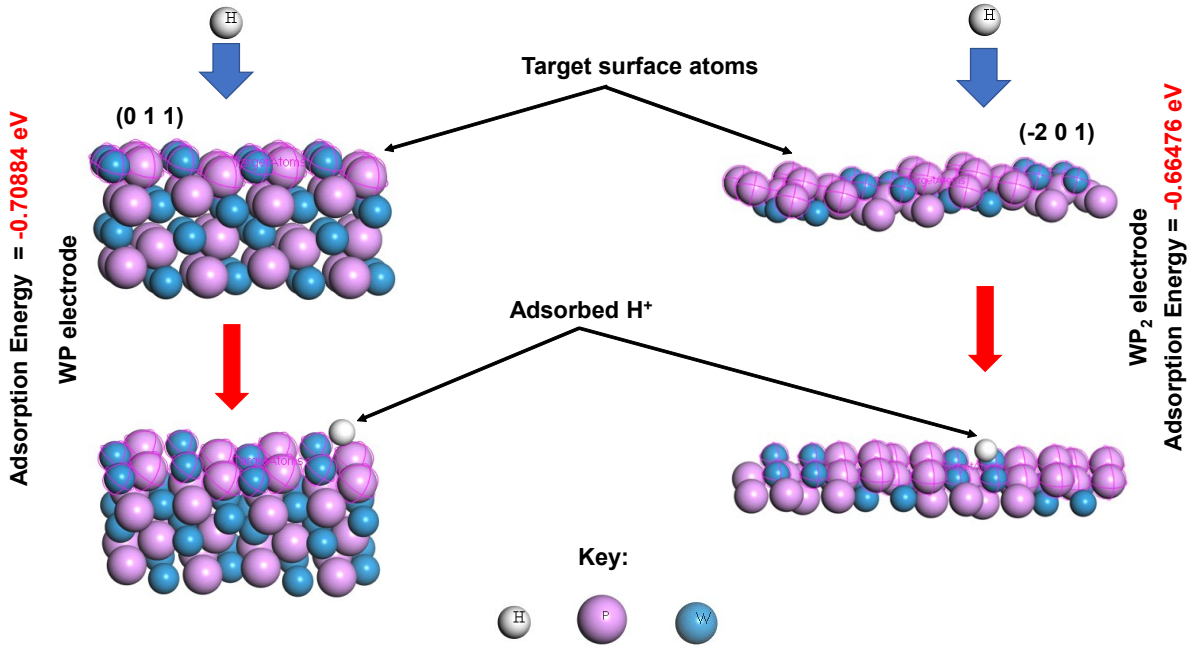


Figure S8: Calculated hydrogen adsorption energies on (011) and (-201) surfaces for WP and α-WP_2, respectively.

Table S3: Calculated adsorption energy using various layer planes of WP and ∝-WP_2.

No. of Layers	Adsorption Energy (eV) (WP)	Adsorption Energy (eV) (∝-WP_2)
1	-0.729952595	-0.690267678
2	-0.74541264	-0.717309001
3	-0.778989849	-0.720332384
4	-0.788683415	-0.720761754

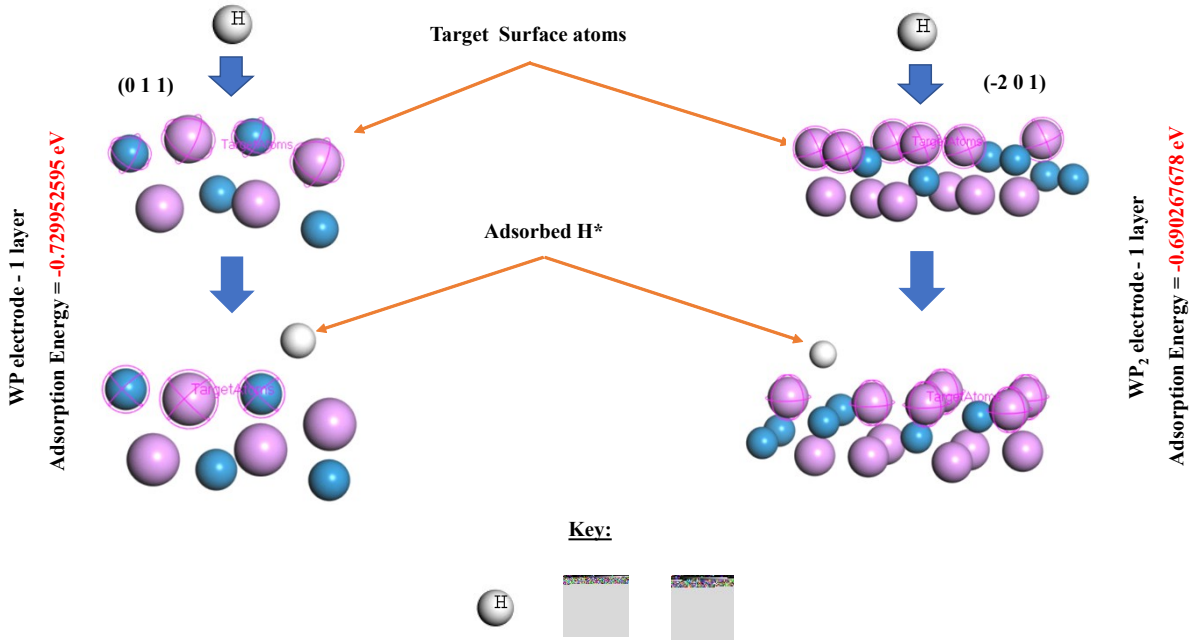


Figure S9: Calculated hydrogen adsorption energies for WP and α-WP_2 using 1-layer.

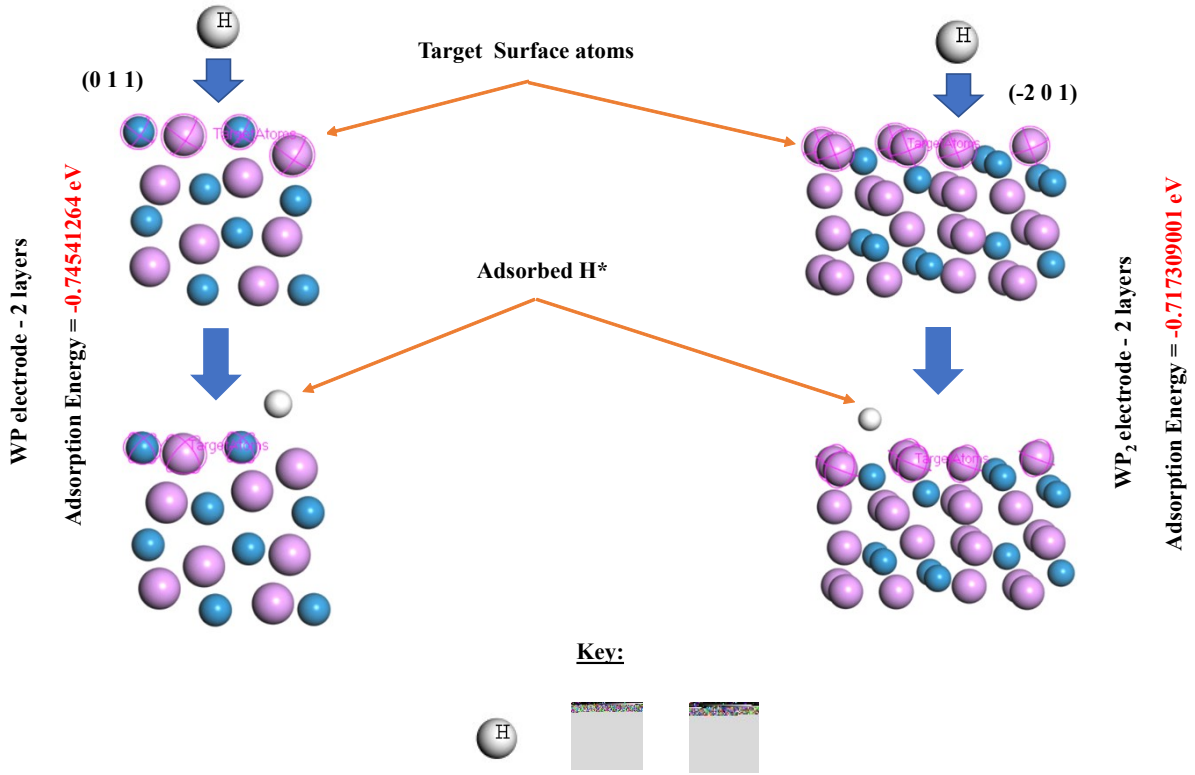


Figure S10: Calculated hydrogen adsorption energies for WP and α-WP_2 using 2-layers.

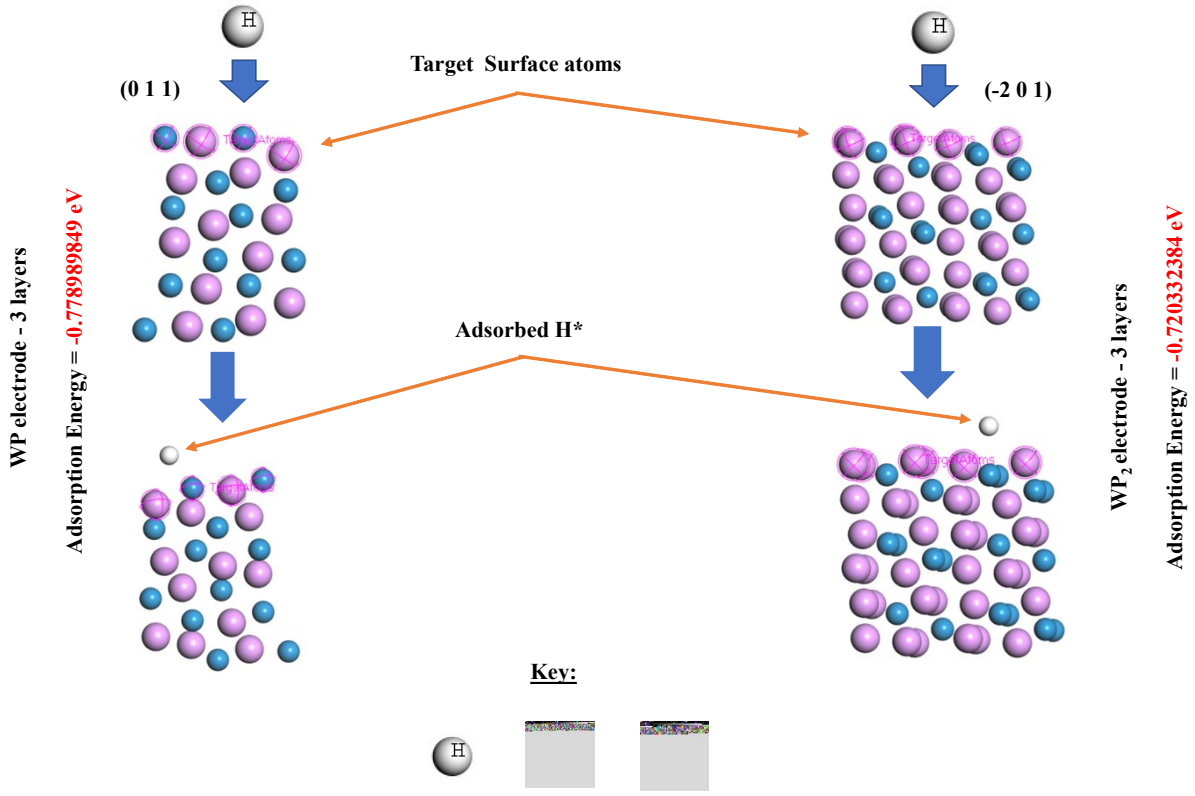


Figure S11: Calculated hydrogen adsorption energies for WP and α-WP_2 using 3-layers.

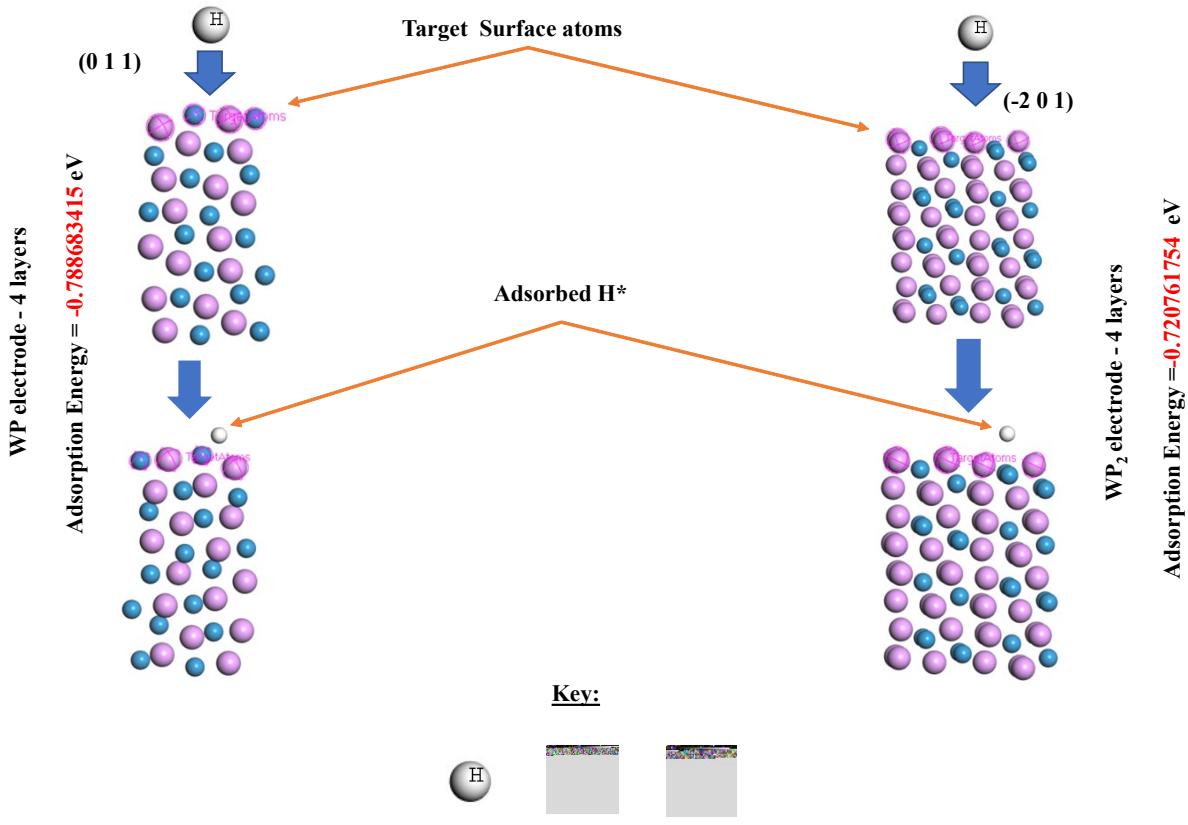


Figure S12: Calculated hydrogen adsorption energies for WP and α-WP_2 using 4-layers.

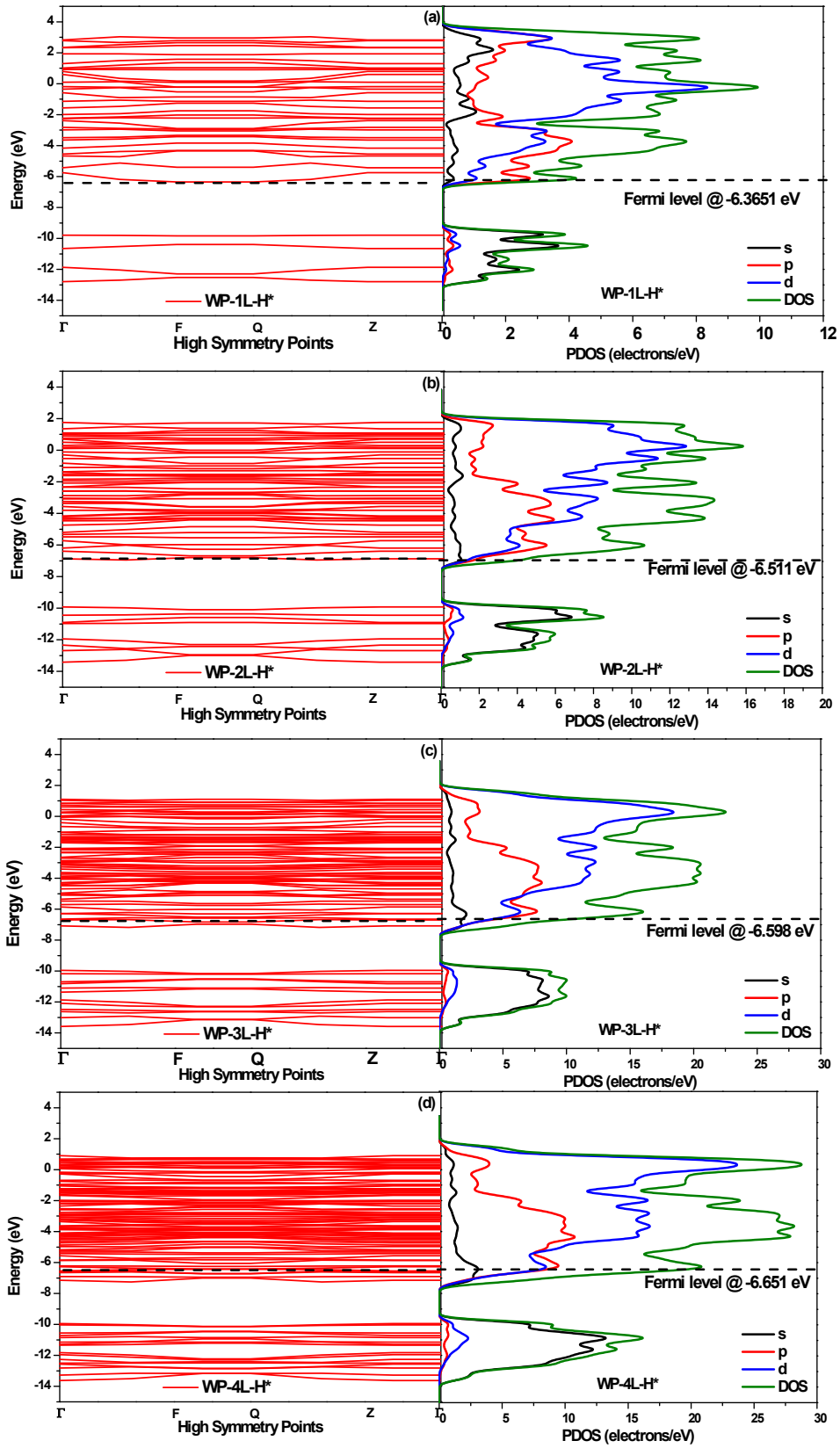


Figure S13: Band structures and DOS plots calculated using (a) 1, (b) 2, (c) 3 and (d) 4 layer planes of the WP (011) surface.

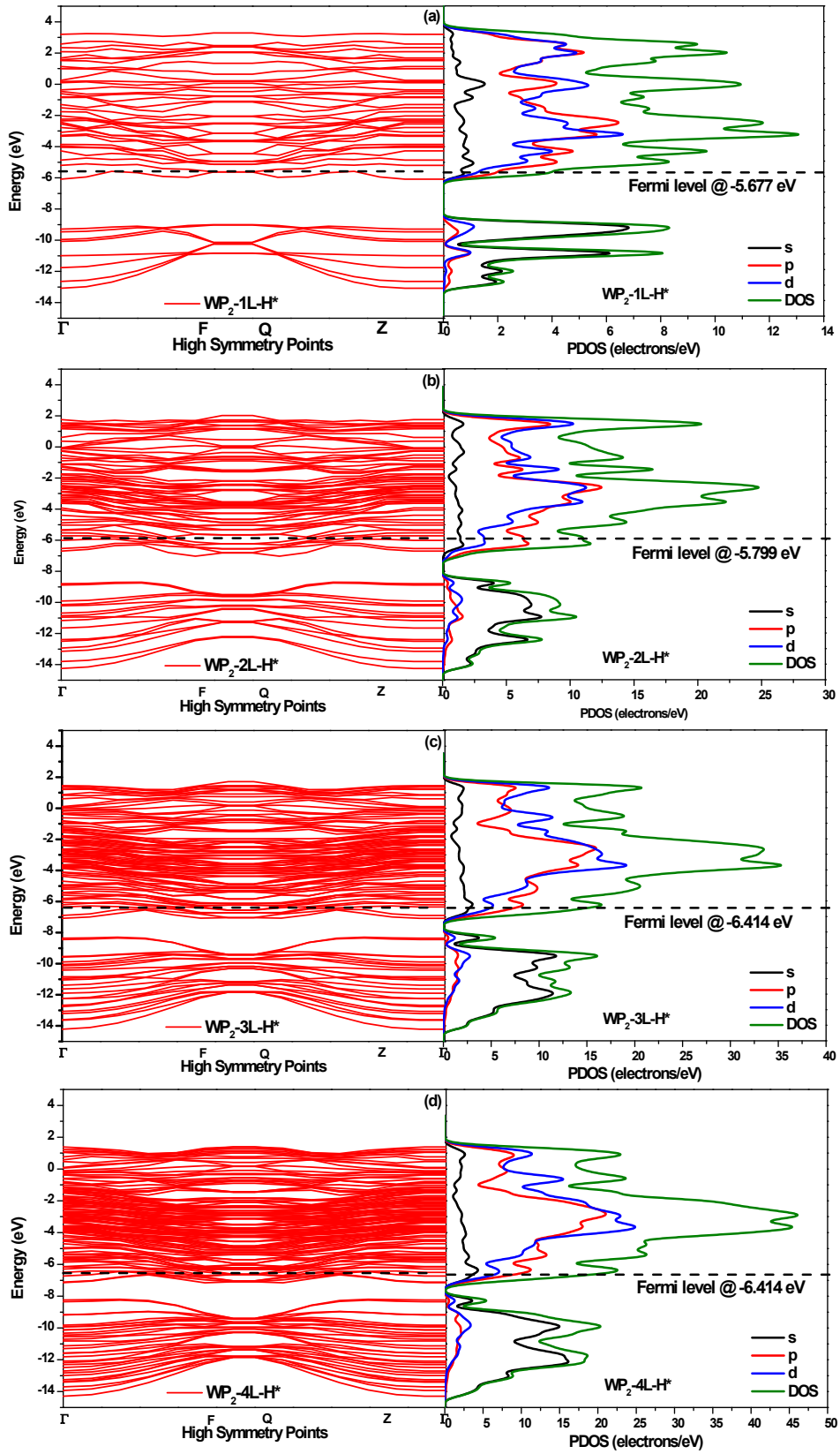


Figure S14: Band structures and DOS plots calculated using (a) 1, (b) 2, (c) 3 and (d) 4 layer planes of the α-WP_2 (-201) surface.

References

1. D. Naveh, E. Towe, Tunable band gaps in bilayer transition-metal dichalcogenides, Physical Review 84 (2011) 205325.
2. S. Ahmad, S. Mukherjee, A comparative study of electronic properties of bulk MoS_2 and its monolayer using DFT technique: Application of mechanical strain on MoS_2 monolayer, Graphene 3 (2014) 52-59.