

Supporting information

A new phosphorene allotrope: the assembly of phosphorene nanoribbons and chains

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Supporting Figure

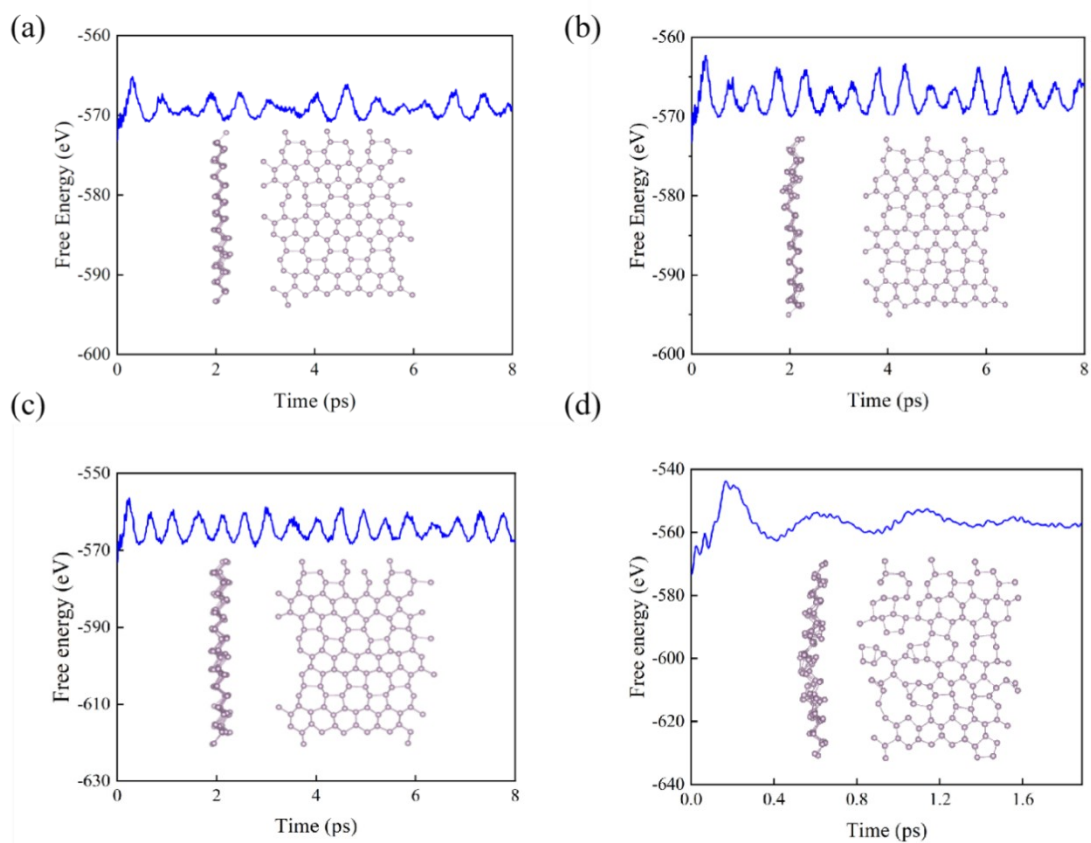


Figure S1. Snapshots of the final frame of the P₅₆₇ monolayer at (a) 300 K, (b) 400 K, (c) 600 K and (d) 1000 K of MD simulations.

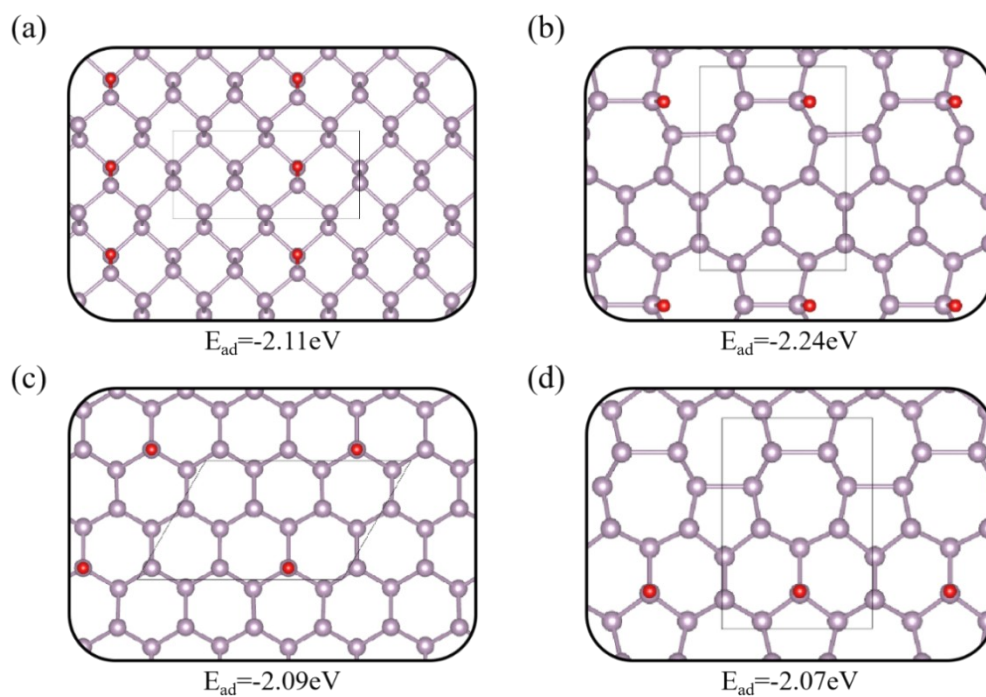


Figure S2. Single oxygen atom adsorption on (a) black phosphorene; (c) blue phosphorene; (b), (d) the P_{567} . The oxygen atoms are in red, and the phosphorus atoms are in purple.

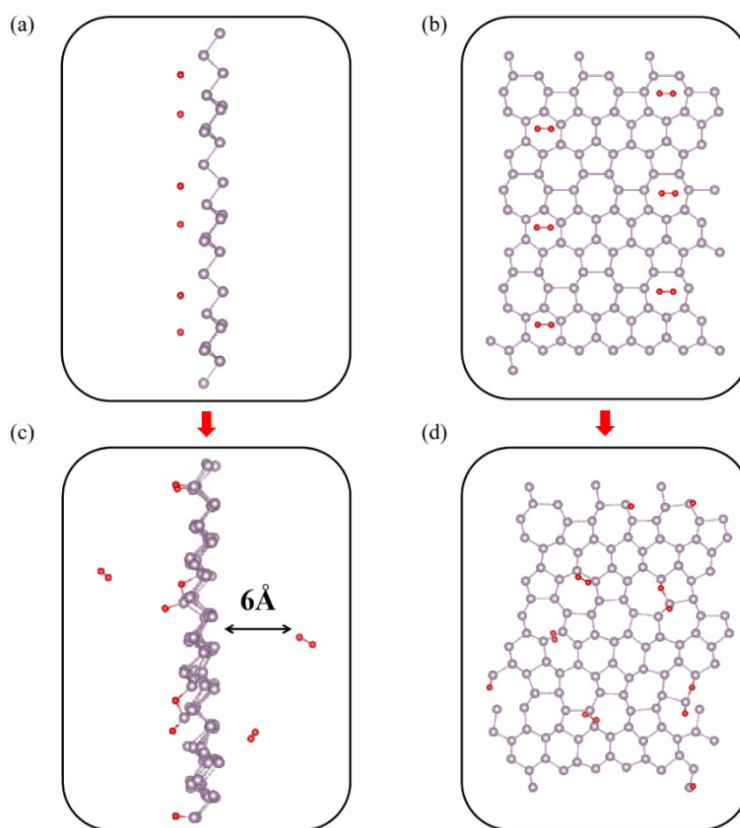


Figure S3. Snapshots after 3 ps MD simulations with temperature controlled at 300 K show the interaction of O₂ with the P₅₆₇.

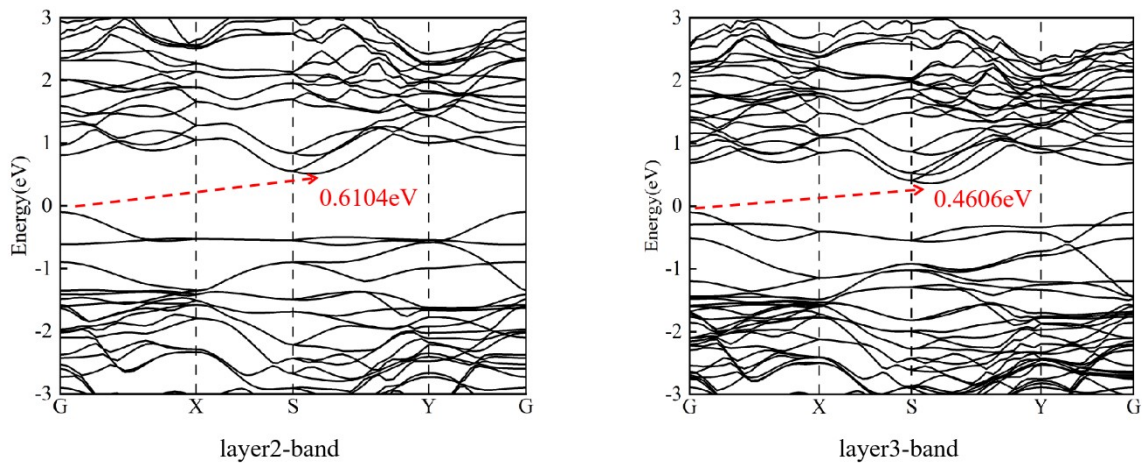


Figure S4. Electronic band structures of the P₅₆₇ multilayers.

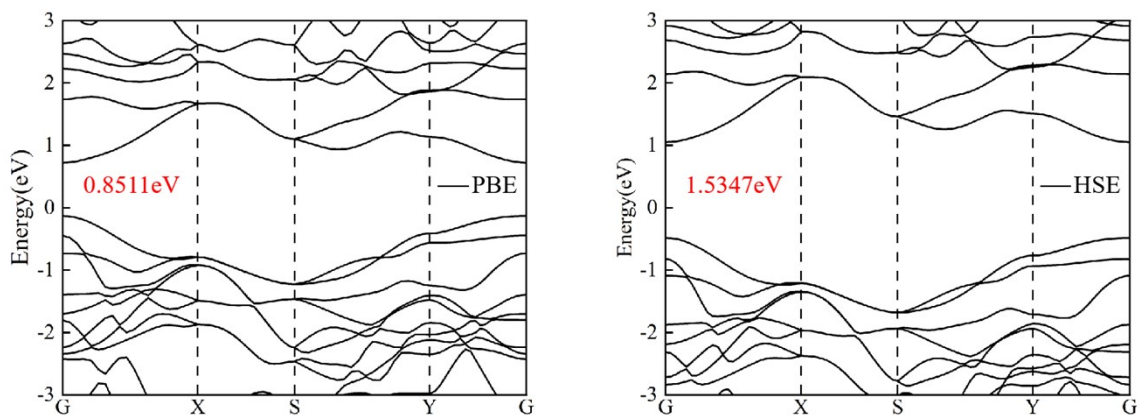


Figure S5. Electronic band structures of the P₅₆₇ monolayer with 10% compression

Supporting Table

Table S1. Effective mass of the P₅₆₇ monolayer and the P₅₆₇ multilayers.

Carrier type	Layer1-m* (m ₀)	Layer2-m* (m ₀)	Layer3-m* (m ₀)
electron (a)	0.457	0.454	0.432
hole (a)	0.527	-0.460	-0.415
electron (b)	0.757	1.285	-0.620
hole (b)	1.165	-0.464	-0.326