Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Fibrous Red Phosphorene: A Promising Two-dimensional Optoelectronic and Photocatalytic Material with Desirable Band Gap and High Carrier Mobility

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Supplementary computational methods

The calculations were performed using the Vienna *Ab initio* Simulation Package (VASP) code, the projector-augmented plane wave (PAW) approach and the Perdew-Burke-Ernzerhof (PBE96) Generalized Gradient Approximation (GGA) density functional.[1-4] In this work, the cutoff energies of 500 eV was set for all compilations. The Brillouin zone was integrated using a regular *k*-point mesh with grid density of $2\pi\times0.02$ Å^{-1}.[5] To achieve more accurate results, the hybrid functional method in the form of Heyd-Scuseria-Ernzerhof (HSE06)[6] is used, and the Grimme's van der Waals (vdW) correction was taken into account to capture the long-range vdW interaction.[7]

References for Supplementary Information

[1] G. Kresse and J. Hafner, *Phys. Rev. B*, 1993, **47**, R558.
[2] G. Kresse and J. Hafner, *Phys. Rev. B*, 1994, **49**, 14251.
[3] G. Kresse and J. Furthmüller, *Comput. Mater. Sci.*, 1996, **6**, 15.
[4] J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865.
[5] J. Monkhorst, J. Pack, *Phys. Rev. B*, 1976, **13**, 5188.
[6] J. Heyd, G. E. Scuseria and M. Ernzerhof, *J. Chem. Phys.*, 2003, **118**, 8207.
[7] S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787.

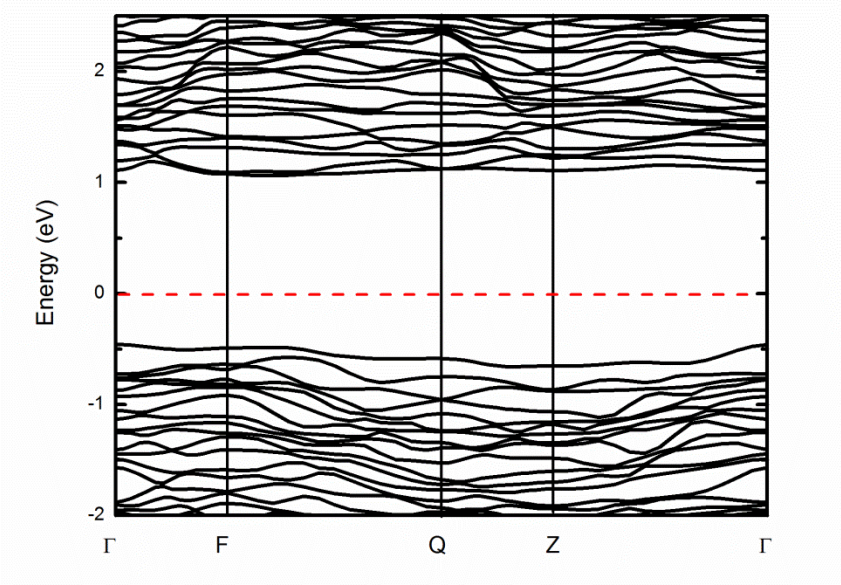

Figure S1 Electronic band structure of bulk fibrous red phosphorus at PBE96 level.

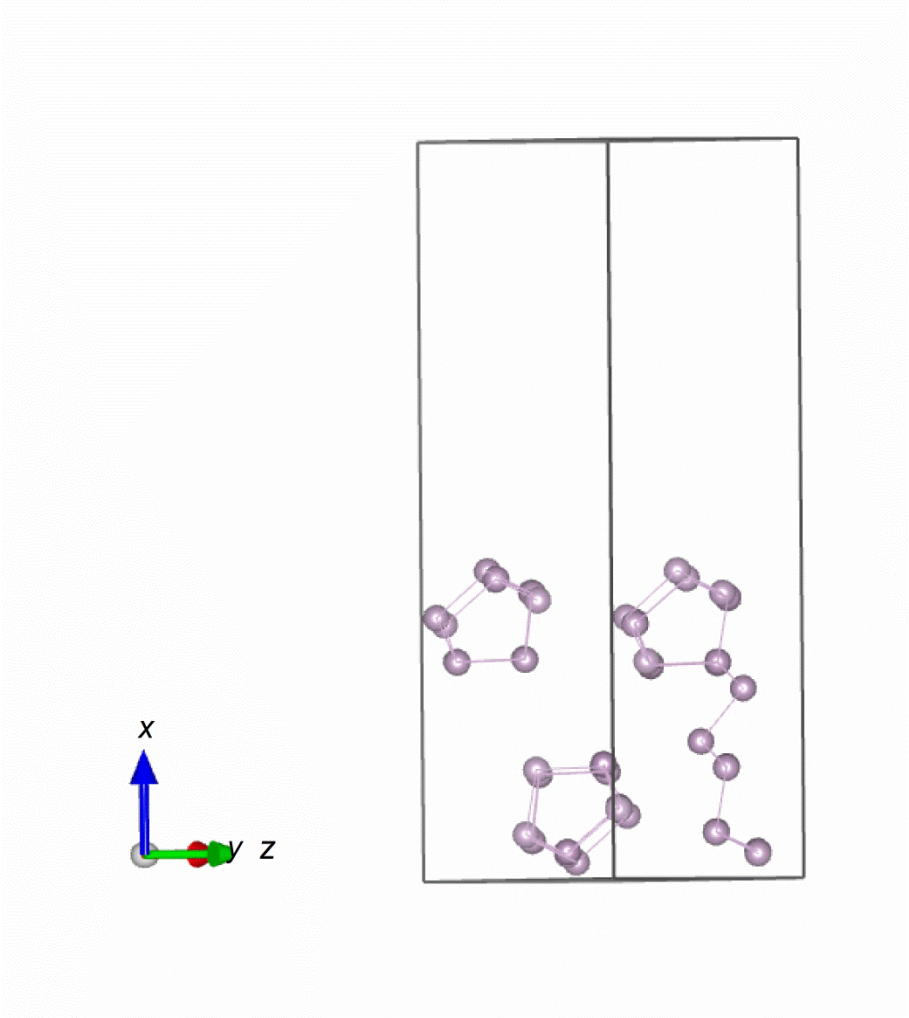

Figure S2 Crystal structure of fibrous red phosphorene monolayer via exfoliating red phosphorus along the *x*-direction.

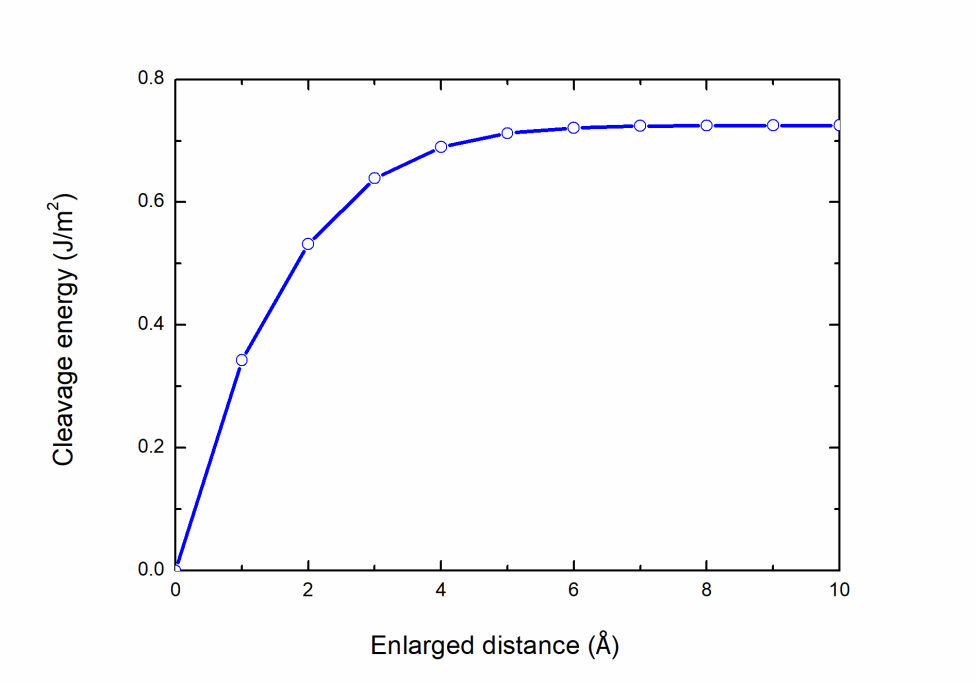

Figure S3 Estimation of cleavage energy for monolayer fibrous red phosphorus along *x*-direction growth from its five-layered slab model.

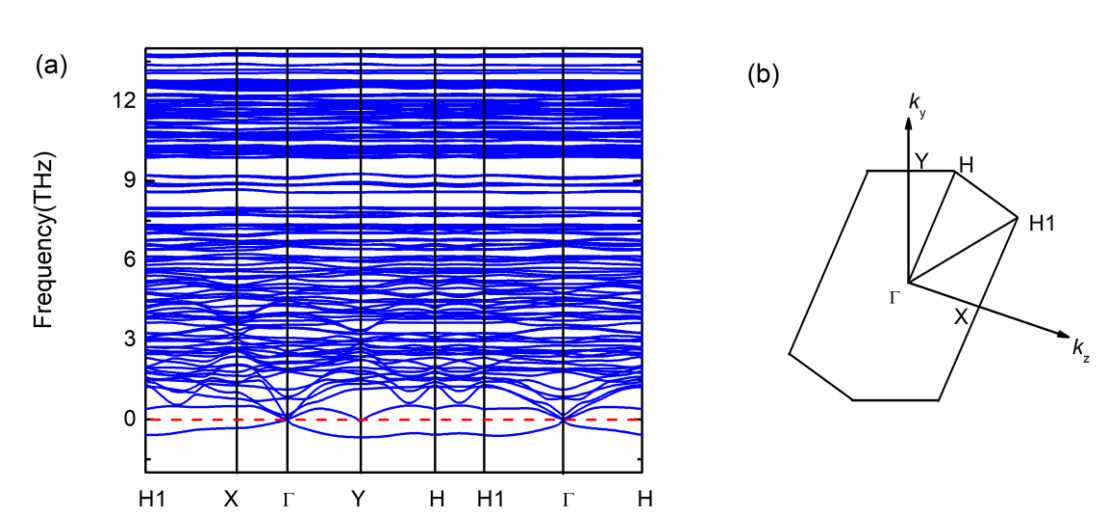

Figure S4 (a) Phonon spectrum of fibrous red phosphorene monolayer along *x*-direction growth. (b) The first Brillouin zone of fibrous red phosphorene monolayer along *x*-direction growth.

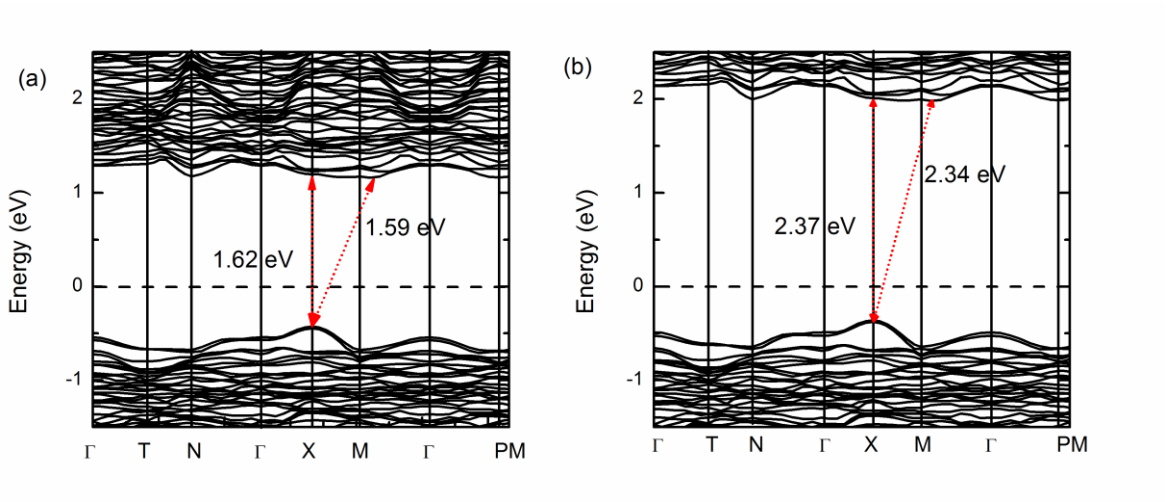

Figure S5 Electronic band structures of fibrous red phosphorene bilayer using (a) standard PBE96 pure functional and (b) advanced HSE06 hybrid functional.

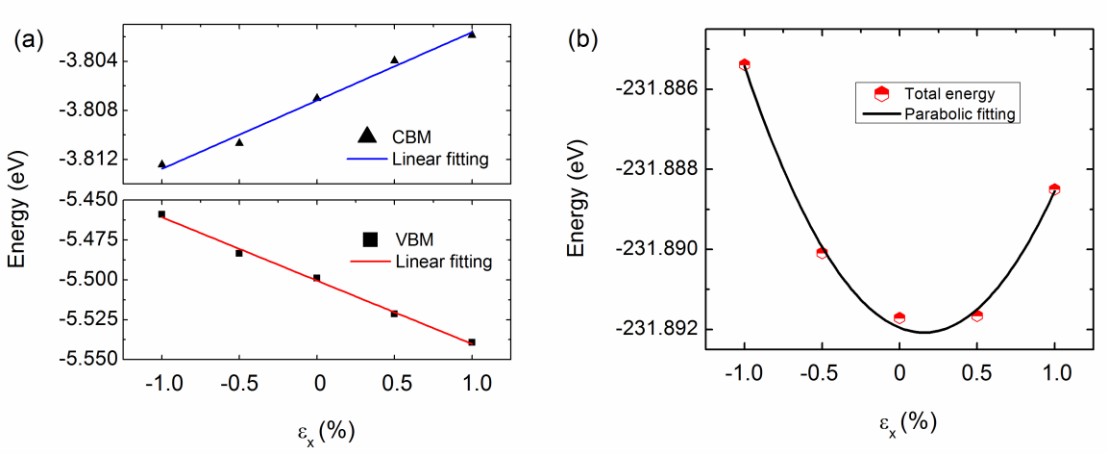

Figure S6 (a) The CBM and VBM of fibrous red phosphorene monolayer with respect to uniaxial strain along the *x* direction. (b) The total energy of fibrous red phosphorene monolayer with respect to uniaxial strain along the *x* direction. The above data were obtained from the PBE96 functional.

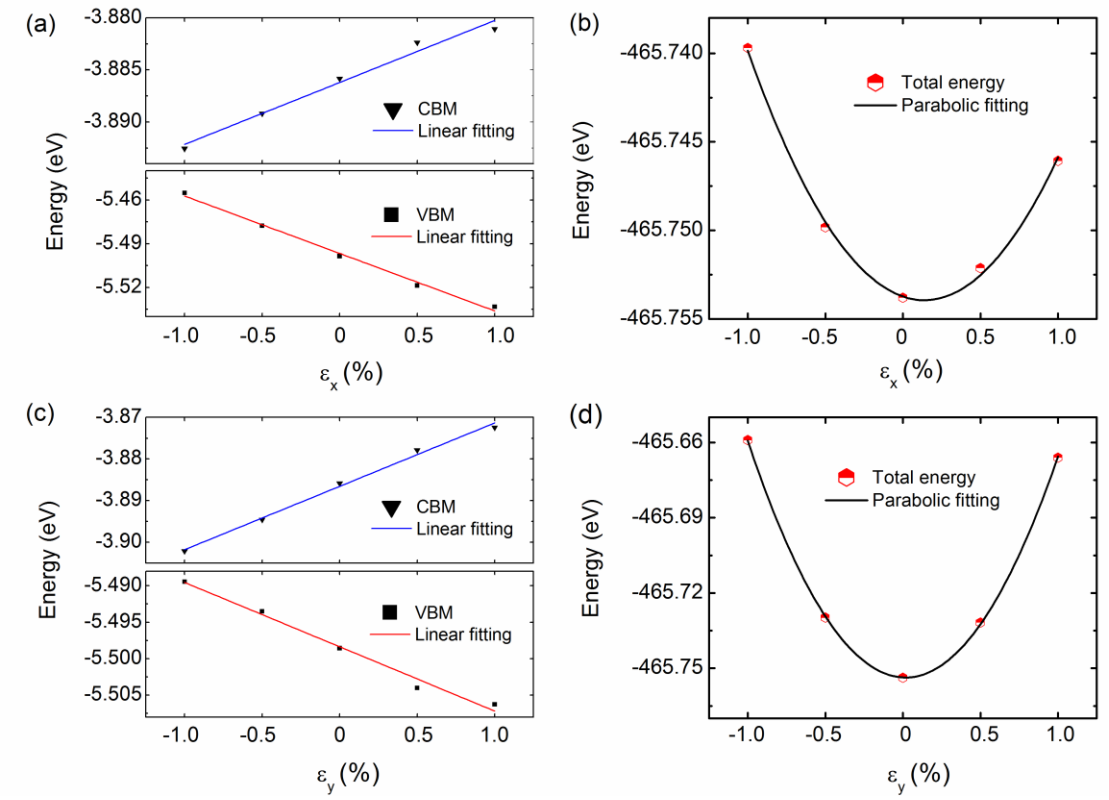

Figure S7 (a) the CBM and VBM of fibrous red phosphorene bilayer with respect to uniaxial strain along the *x* direction. (b) The total energy of fibrous red phosphorene bilayer with respect to uniaxial strain along the *x* direction. (c) The CBM and VBM of fibrous red phosphorene bilayer with respect to uniaxial strain along the *y* direction, (d) the total energy of fibrous red phosphorene bilayer with respect to uniaxial strain along the *x* direction. The above data were obtained from the PBE96 functional.

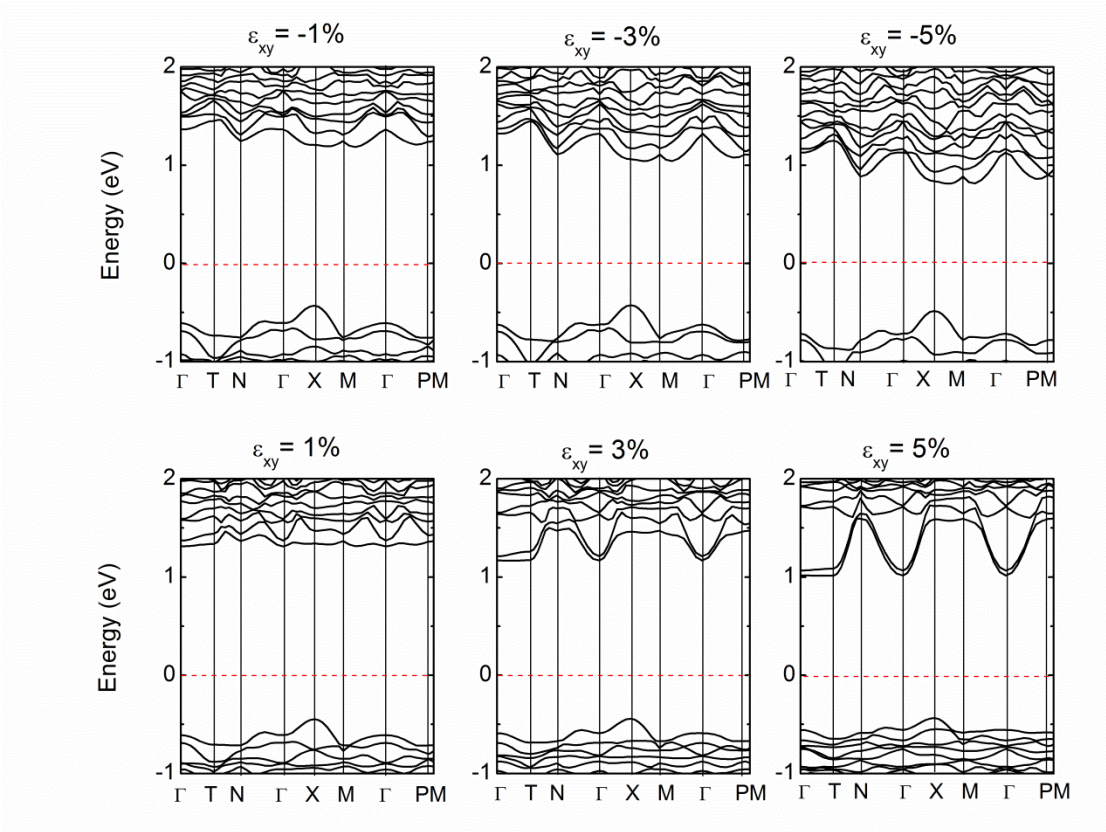

Figure S8 Electronic band structures of fibrous red phosphorene monolayer upon different in-plane biaxial strains obtained from the PBE96 functional.

Table S1 Predicted effective mass (m*), deformation potential (E_1, in eV), 2D elastic modulus (C^{2D}, in J/m^2), and electron and hole mobility (μ^{2D}, in 10^3 cm^2 V^{-1} s^{-1}) along the x and y directions for fibrous red phosphorene bilayer.

Carrier type	m_x^* / m_0	m_y^* / m_0	E_{1x}	E_{1y}	C_{x_2D}	C_{y_2D}	μ_{x_2D}	μ_{y_2D}
electrons	0.43	0.58	3.94	0.88	21.82	183.16	0.14	17.2
holes	2.95	0.44	0.60	1.52	21.82	183.16	0.39	3.37