Supporting Information

Structural, elastic, electronic and optical properties of novel tricycle-like phosphorenes

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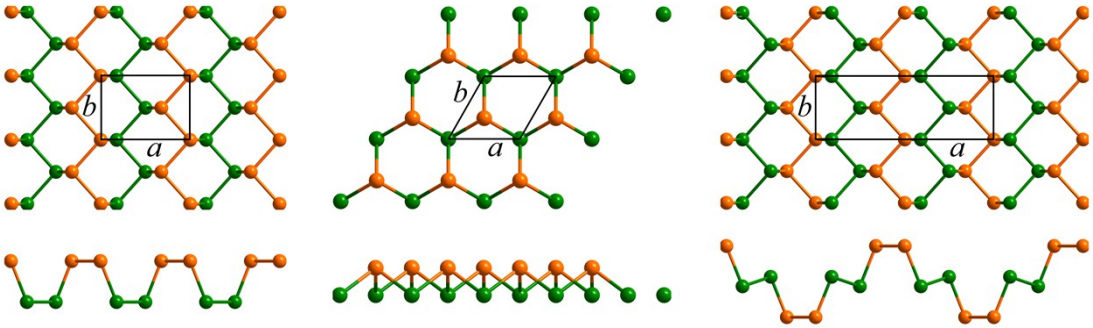
Supporting Figures:



(a) Black phosphorene (b) Blue phosphorene (c) Red phosphorene

Fig. S1 Optimized structures viewed from top and side directions for (a) black, (b) blue, and (c) red phosphorenes. Orange and green balls represent P atoms in different atomic planes. Unit cell is shown in black solid lines.

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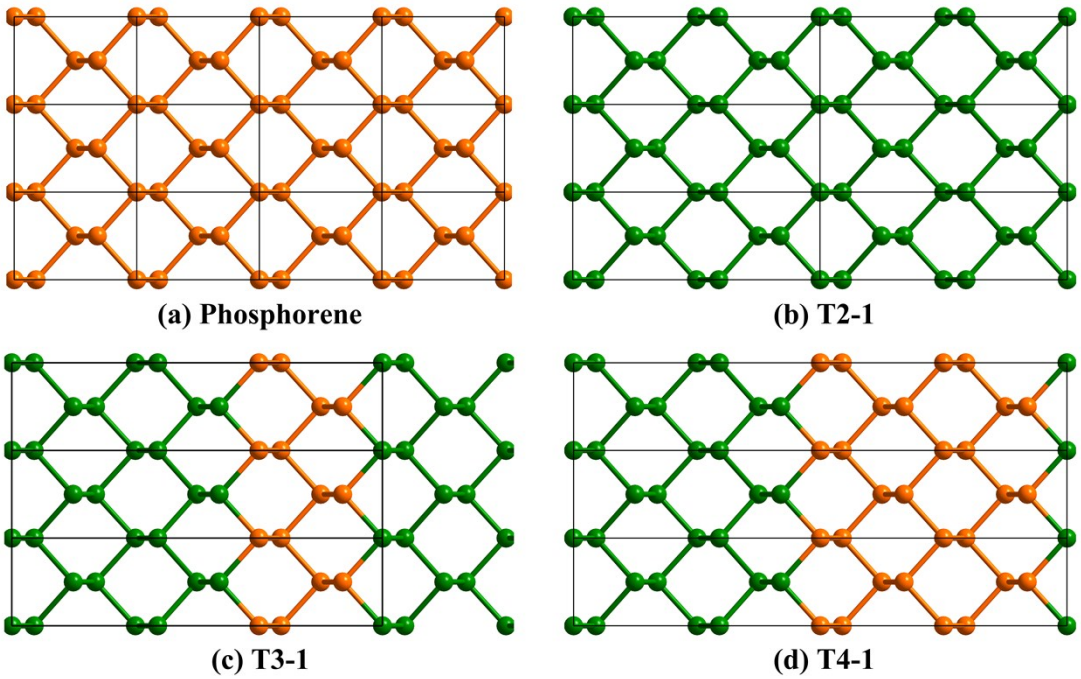

Fig. S2 Optimized structures viewed from top direction for (a) 4 × 3 black phosphorene, (b) 2 × 3 T2-1, (c) 1 × 3 T3-1, and (d) 1 × 3 T4-1. Orange and green balls represent P atoms in the regions of black and red phosphorene structures, respectively. Unit cell is denoted as black solid lines.

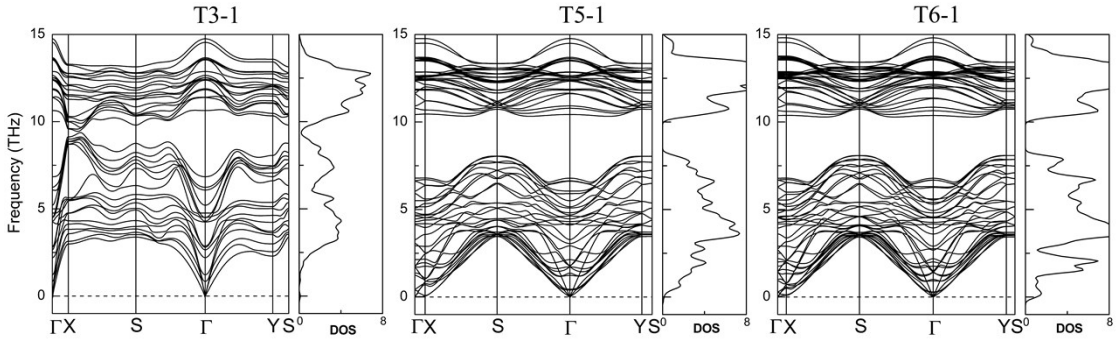

Fig. S3 Phonon spectrum and density of state (DOS) of hybrid phosphorenes. The phonon spectrum and DOS are calculated by using the PHONON software, which is confirmed to be valid for exploring the two-dimensional nanomaterials. A large supercell size (close to or over 10 Å) is adopted along both armchair and zigzag directions. A displacement of 0.05 Å is used to calculate the Hellmann-Feynman forces in the supercell by VASP. Subsequently, the PHONON software is employed to construct the dynamic matrix and the derivatives of the dielectric constant tensor, where the related information of phonon spectrum can be analyzed.

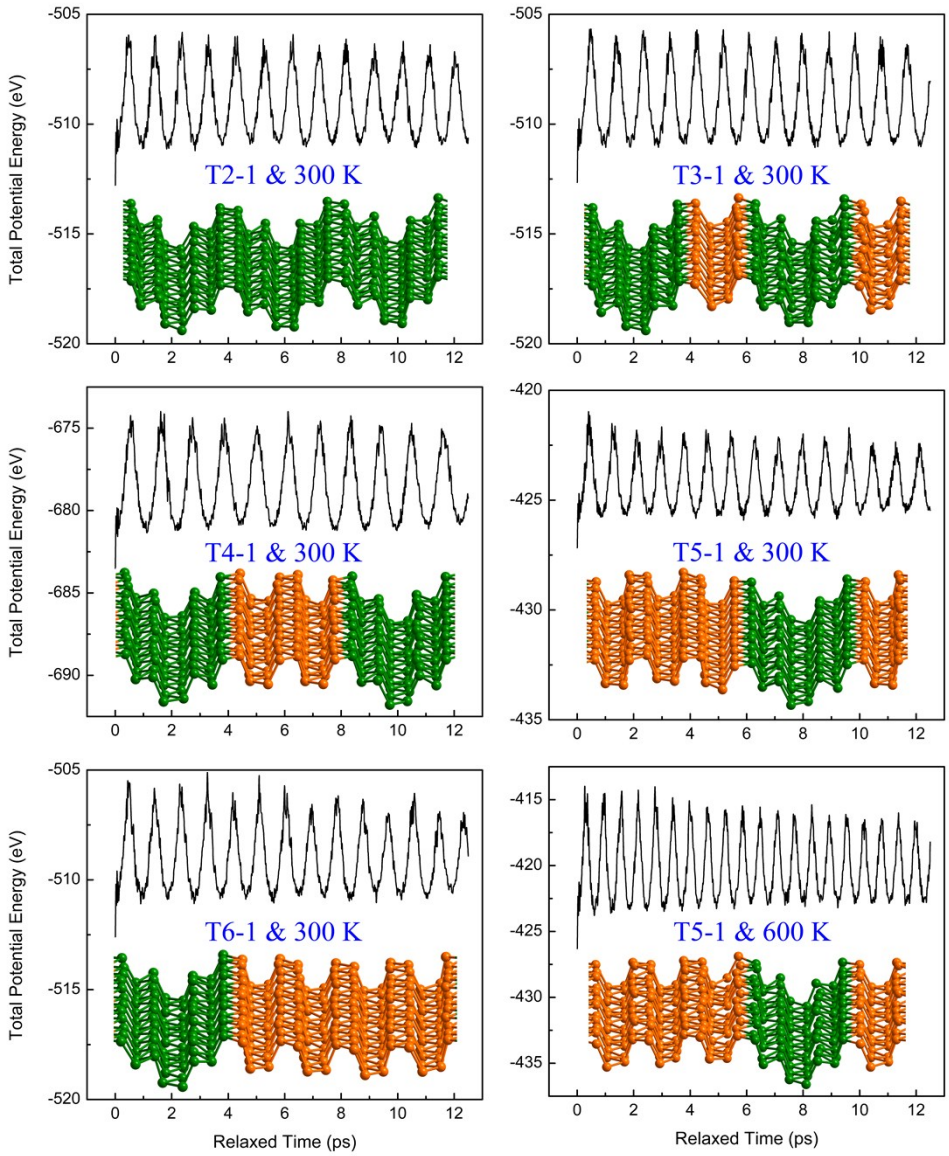

Fig. S4 The vibrations of total potential energy of hybrid phosphorene vs. the relaxed time performed by the *ab initio* molecular dynamical simulations. The inset show the snapshots of the hybrid phosphorenes. *Ab initio* molecular dynamical (MD) simulations have been performed at the temperature of 300 or 600 K with a time step of 3.0 fs. A large rectangular supercell (the size along armchair direction is over than 23 Å, and along zigzag direction is over than 13 Å) is employed to minimize the constraint induced by periodic boundary conditions. After running 12.5 ps, geometrical structures of all the hybrid phosphorenes are still sustained with slight distortion, indicating that these hybrid phosphorenes are dynamical stable at the room temperature.

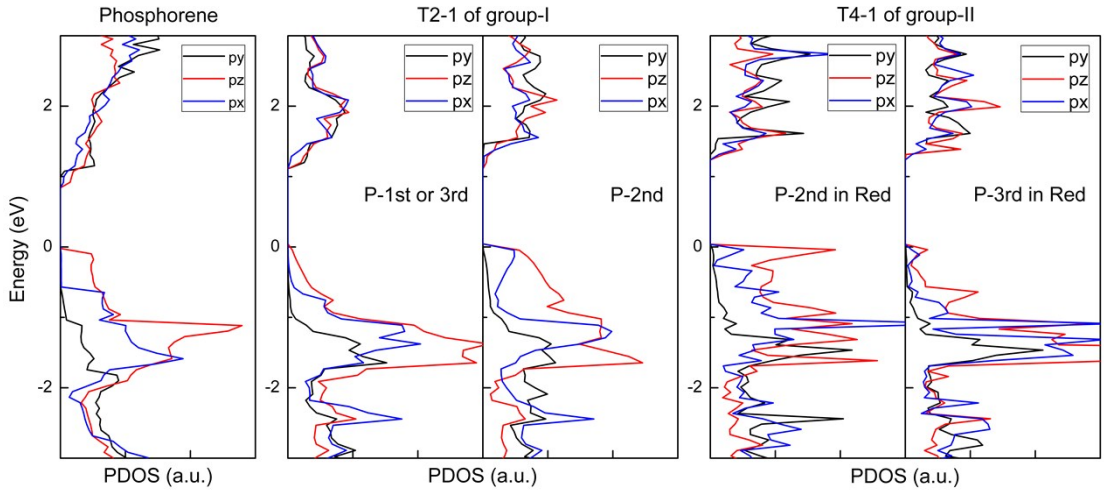

Fig. S5 Partial density of states (PDOS) of the black and hybrid phosphorenes. "1st, 2nd, and 3rd" denote different atomic planes marked out in Fig. 1, and "Red" represents P atom in the region of red phosphorene structure.

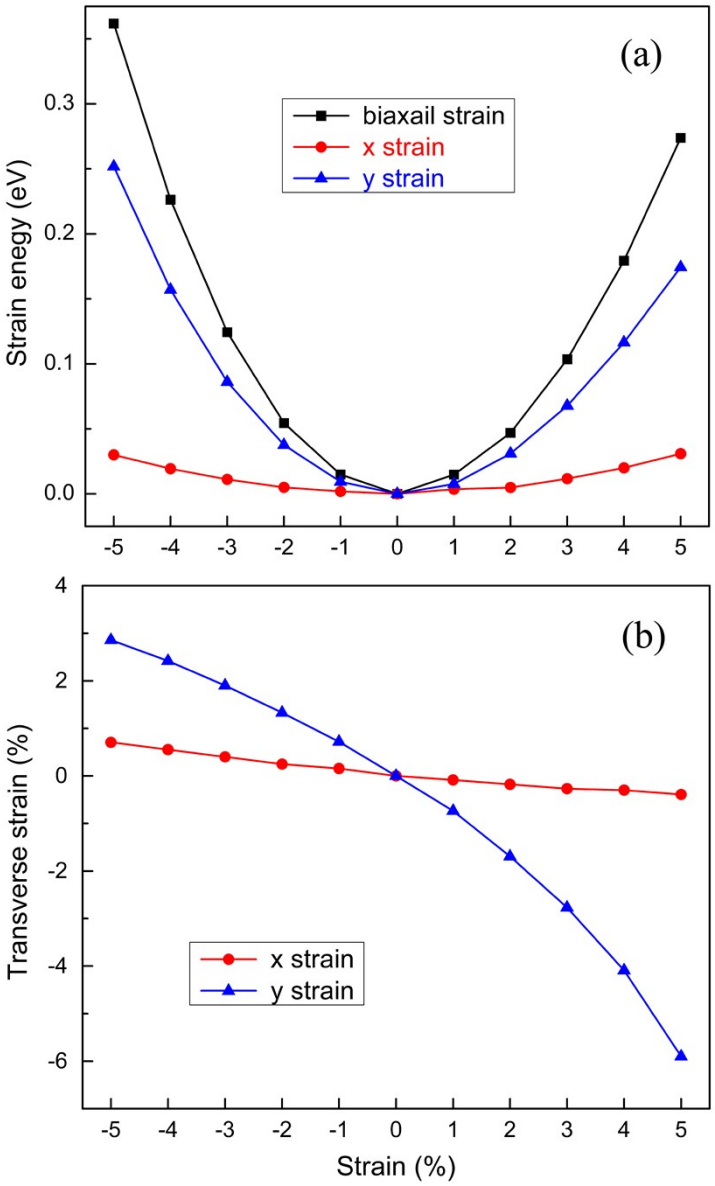

Fig. S6 Strain energy (a) and transverse strain (b) of T2-1 as a functional of various in-plane strains. Uniaxial *x* and *y* strains are applied along the armchair and zigzag directions, respectively.

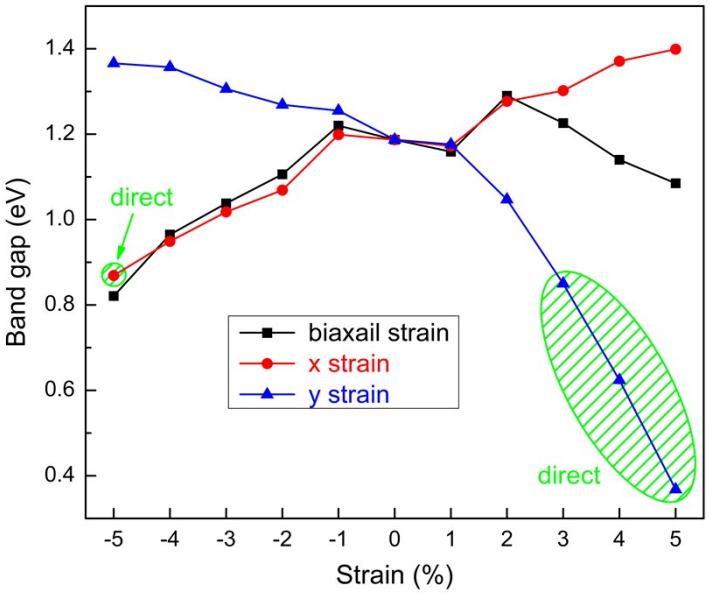

Fig. S7 Band gap of T2-1 as a functional of various in-plane strains. Uniaxial *x* and *y* strains are applied along the armchair and zigzag directions, respectively.

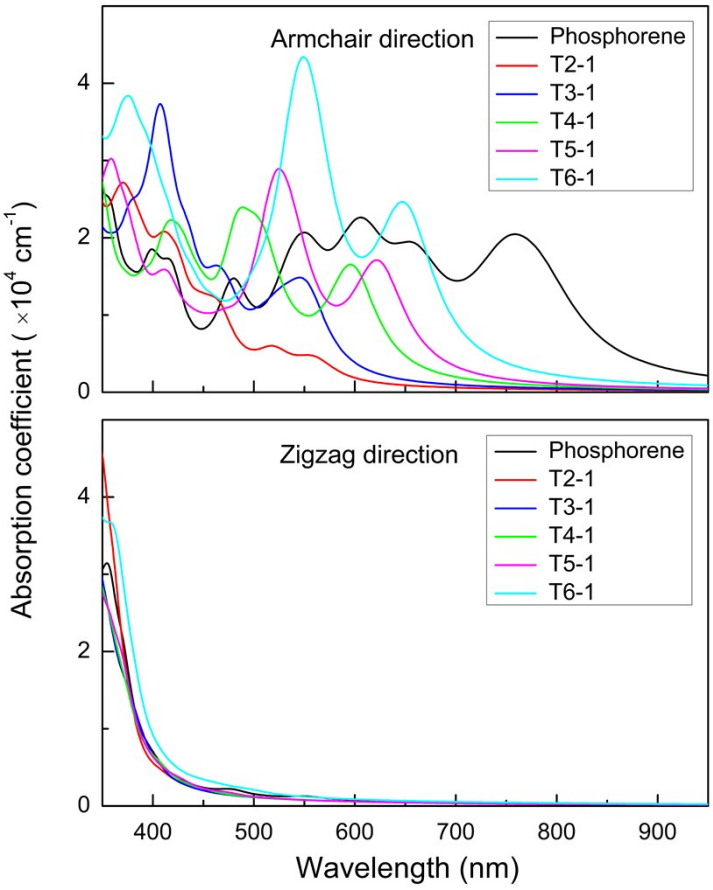

Fig. S8 Spectra of optical absorption coefficient of the black and hybrid phosphorenes along armchair and zigzag directions calculated by time-dependent DFT (TDDFT).