Supporting Information

for

Partially Planar BP_3 with High Electron Mobility as a Phosphorene Analog

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Mechanical Properties

Herein, we describe the mechanical properties of the 2D sheets, which can be quantified by two independent parameters, i.e., the in-plane stiffness C and Poisson's ratio ν. In-plane stiffness can be calculated from the second derivative of the strain energy with respect to strain using the formula: $C = (1/S_0)(\partial^2 E_s/\partial\varepsilon^2)$, where S_0 is the equilibrium area of the primitive cell. The strain energy is defined by the relation: $E_s = E_\varepsilon - E_0$, where E_ε is the total energy of the strained system, and E_0 is the corresponding energy in equilibrium. ε is the uniaxial strain defined by the relation: $\varepsilon = \frac{(a' - a_0)}{a_0} \times 100$, where a' and a_0 are the lattice constants of strained and unstrained systems, respectively. Poisson's ratio ν is defined by the relation: $\nu = -\frac{\varepsilon_{trans}}{\varepsilon_{axial}}$, where ε_{axial} and ε_{trans} are the strain along the direction of the stress and that perpendicular to the stress, respectively. Note that ε_{trans} is negative, because the sheet tends to be compressed in the direction perpendicular to the applied stress.

The elastic parameters of an anisotropic 2D material are calculated using the harmonic approximation: $E_s = p_{11}\varepsilon_X^2 + p_{12}\varepsilon_Y^2 + p_2\varepsilon_X\varepsilon_Y$, where ε_X and ε_Y are strains along the X- and the Y-axis, respectively. In total, 25 (ε_X,ε_Y) points are selected in the range of -1.5 %$\leq \varepsilon_i \leq$1.5 % (i = X,Y) in such a manner that the incremental value of ε_i is 0.75. A full structure optimization was performed at each strain. p_{11} , p_{12} , and p_2 can be determined from surface fitting to the harmonic equation. Finally, in-plane stiffness parameters along the two directions (C_X and C_Y) as well as Poisson's ratios (ν_X and ν_Y) can be calculated from the relations: $C_X = (2p_{11} - p_2^2/2p_{12})/S_0$, $C_Y = (2p_{12} - p_2^2/2p_{11})/S_0$, $\nu_X = p_2/2p_{12}$, and $\nu_Y = p_2/2p_{11}$.

Table S1. Various parameters for stacking patterns of the bilayer of the α BP_3 other than three most stable ones.

Stacking pattern	(a,b)[a]	E_{rel} (eV/supercell)[b]
AG[c]	3.23,5.50	0.002
AE'[d]	3.24,5.50	0.002
AH[e]	3.23,5.49	0.025
AD'	3.24,5.50	0.038
AC'	3.24,5.50	0.044
AF	3.23,5.49	0.055
AB[f]	3.23,5.49	0.058
AD[f]	3.23,5.49	0.058
AI[f]	3.24,5.50	0.058
AA'	3.24,5.50	0.143

[a]Two lattice parameters in Å unit.
[b]The relative energy is defined with respect to that of AA stacking pattern in eV per supercell composed of eight atoms.
[c]The pattern relaxes to the one similar to AA after structure optimization.
[d]The pattern relaxes to the one similar to AB′ after structure optimization.
[e]The pattern relaxes to the one similar to AC after structure optimization.
[f]The three initial patterns relax to the same final one after structure optimization.

Figure S1. Chemical structures of two less stable phases (a and b) of the BP_3 monolayer. Two different views are shown for each of them.

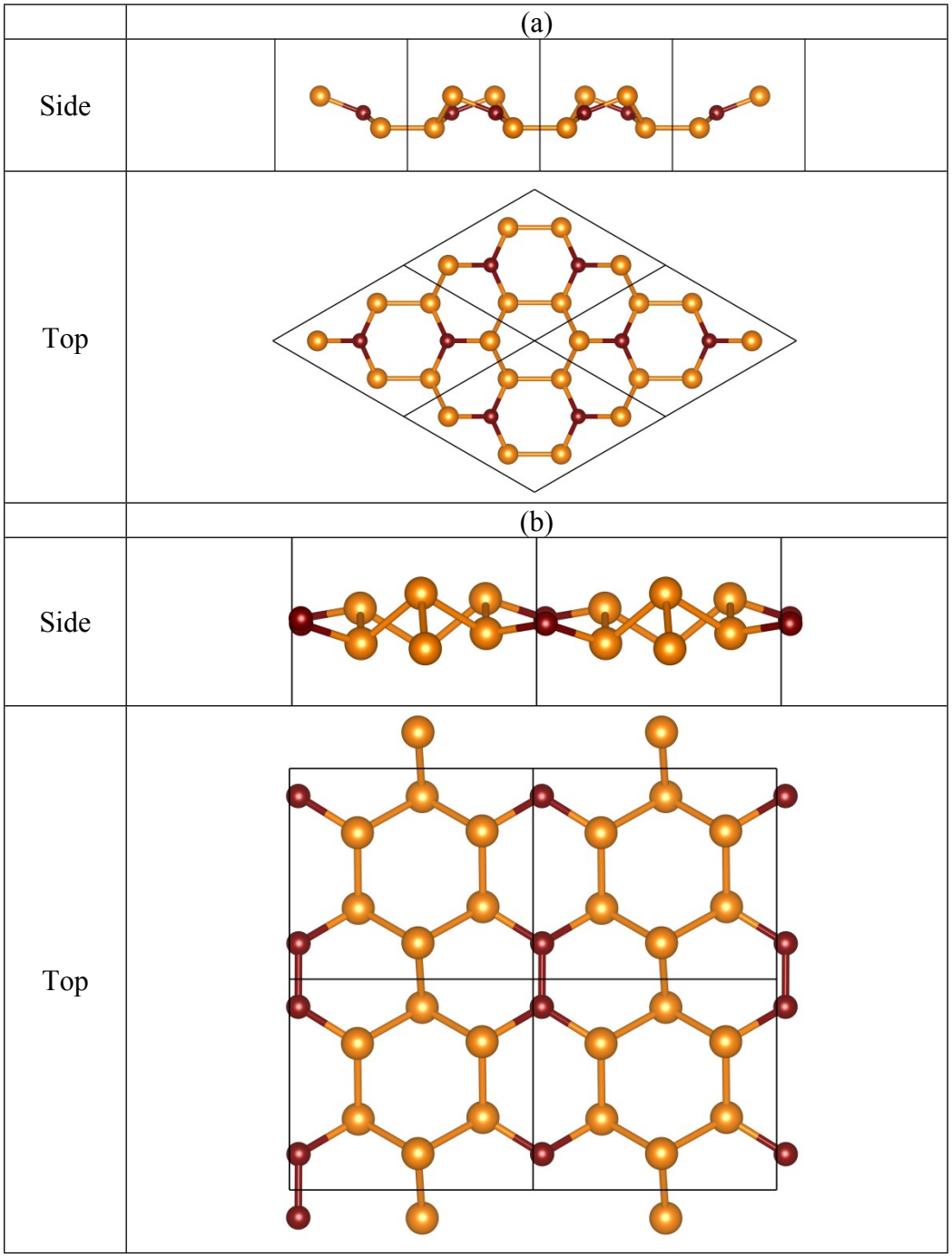
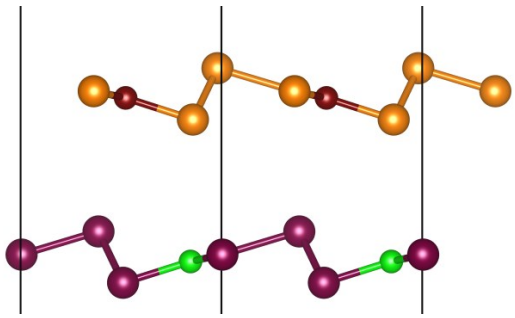
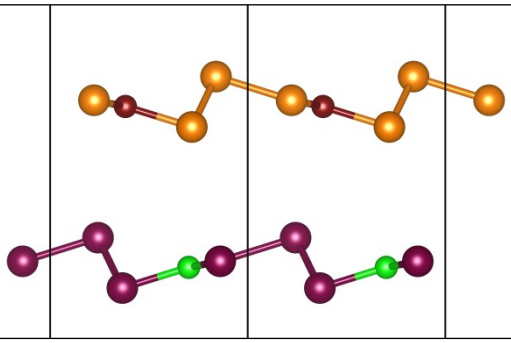
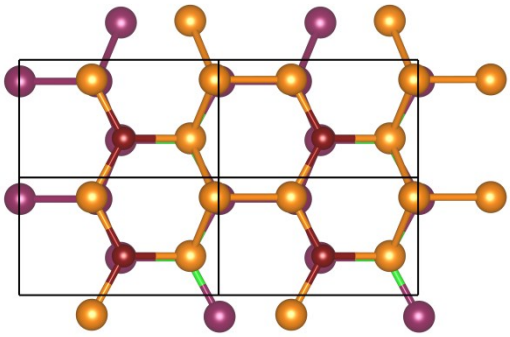
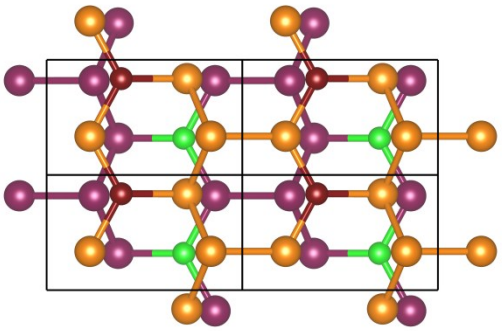
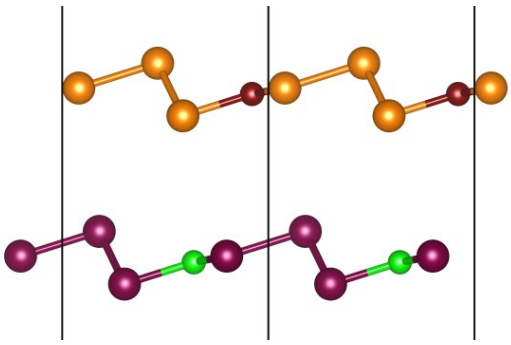
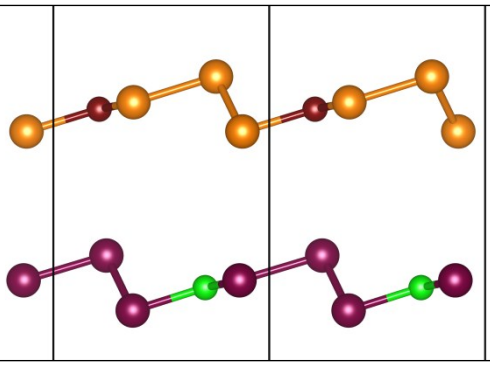
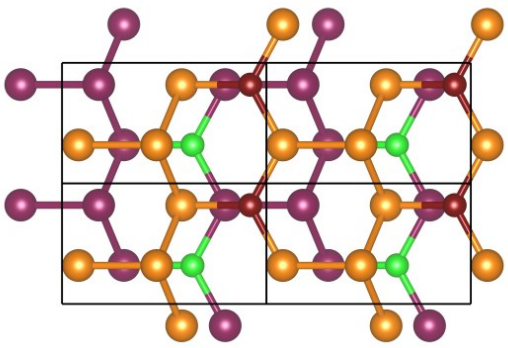
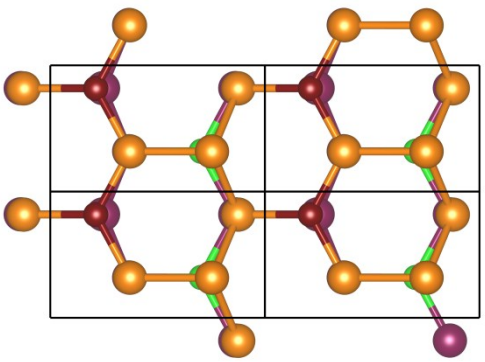


Figure S2. Chemical structures of various stacking patterns of the α BP_3 bilayer other than three most stable ones shown in Table S1. Two different views are shown for each of them.

	AD'	AC'
Side		
Top		

	AF	AD
Side		
Top		

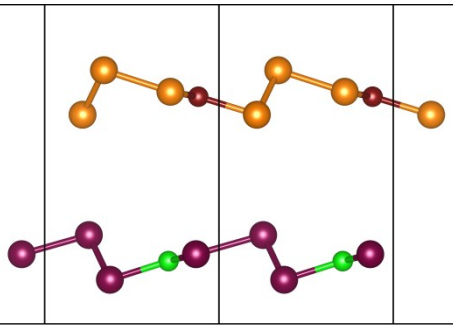
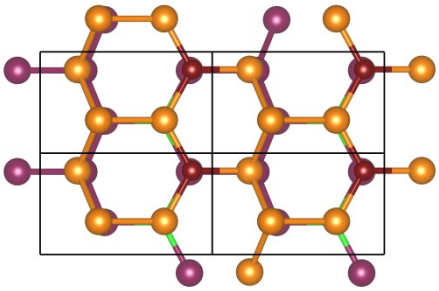
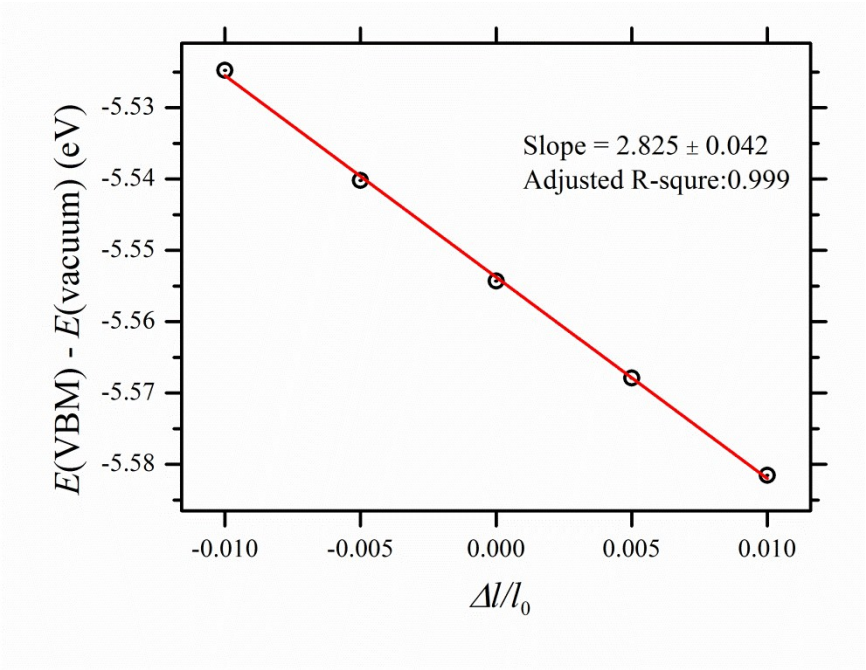
	AA'	
Side		
Top		

Figure S3. Energy eigenvalues of the VBM (a) and CBM (b) of the α BP_3 monolayer with respect to the vacuum level as functions of the lattice dilation $\Delta l / l_0$ along the zigzag direction. For each of them, a least square fit and its standard deviation are also shown.

(a)



(b)

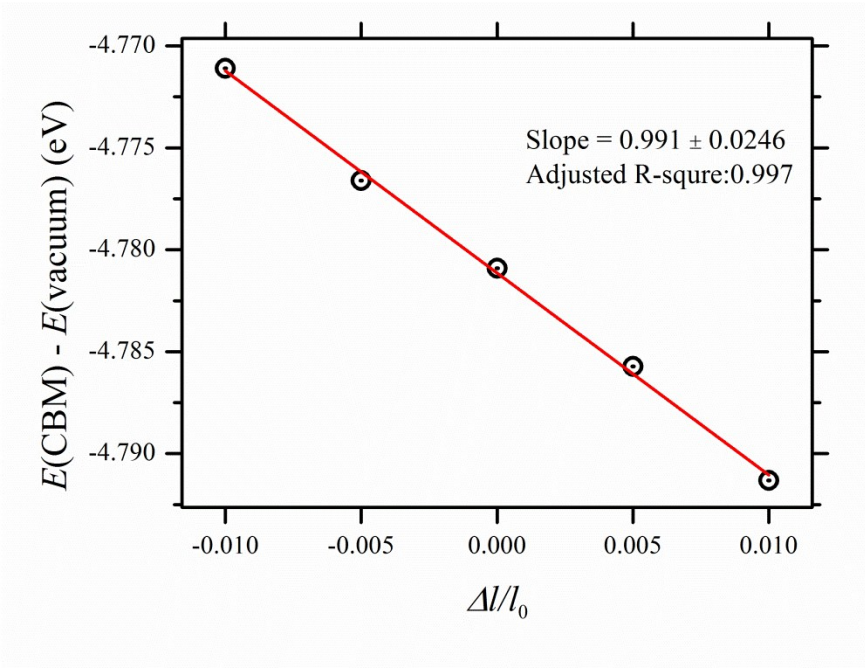
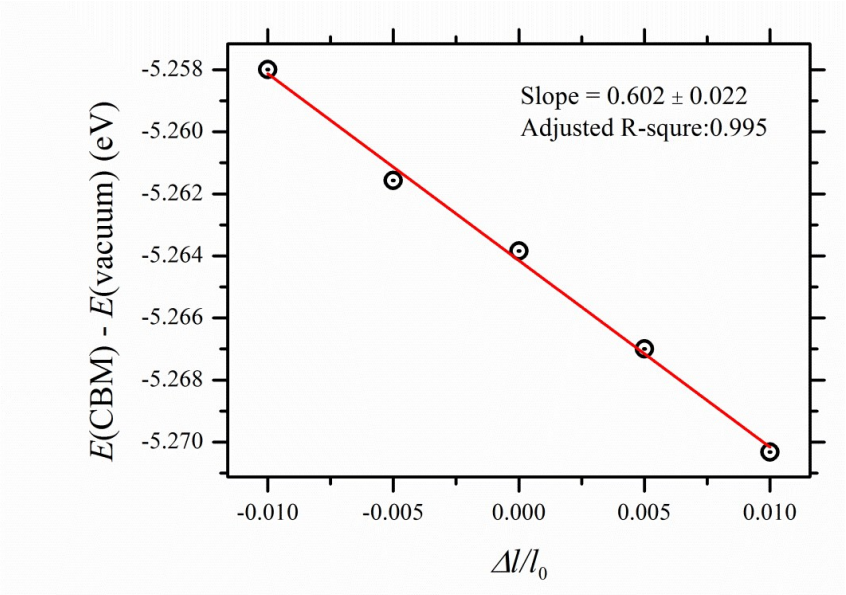


Figure S4. Energy eigenvalues of the CBM of patterns AA (a) and AB' (b) with respect to the vacuum level as functions of the lattice dilation $\Delta l / l_0$ along the zigzag direction. For each of them, a least square fit and its standard deviation are also shown.

(a)



(b)

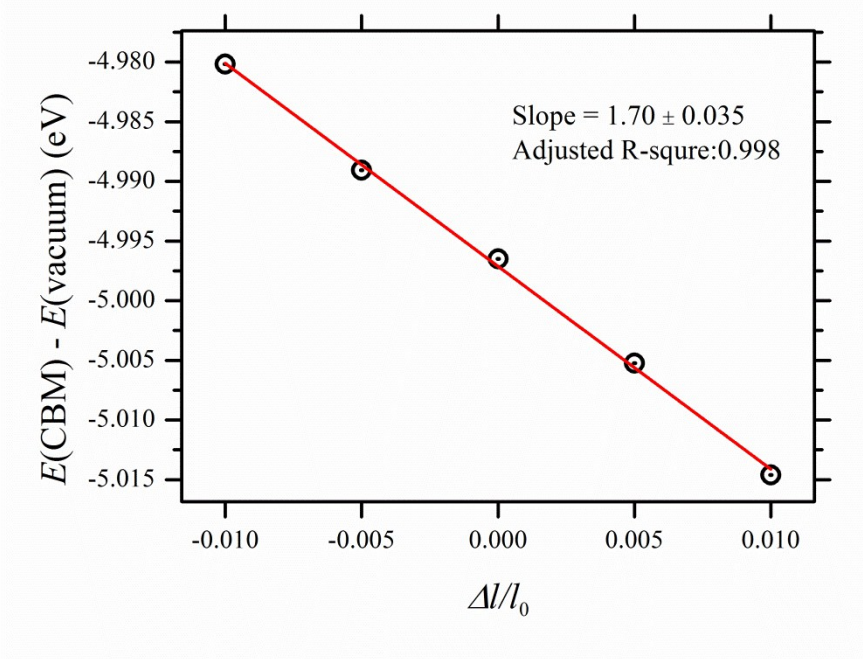
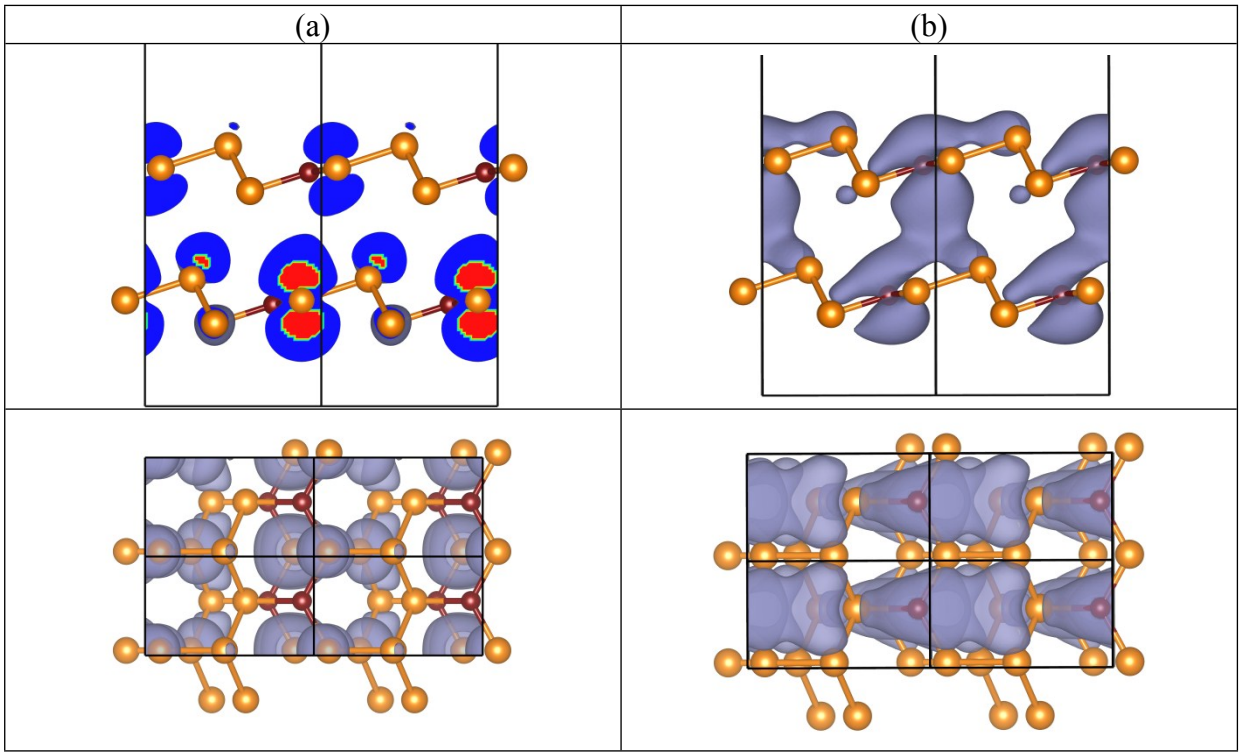
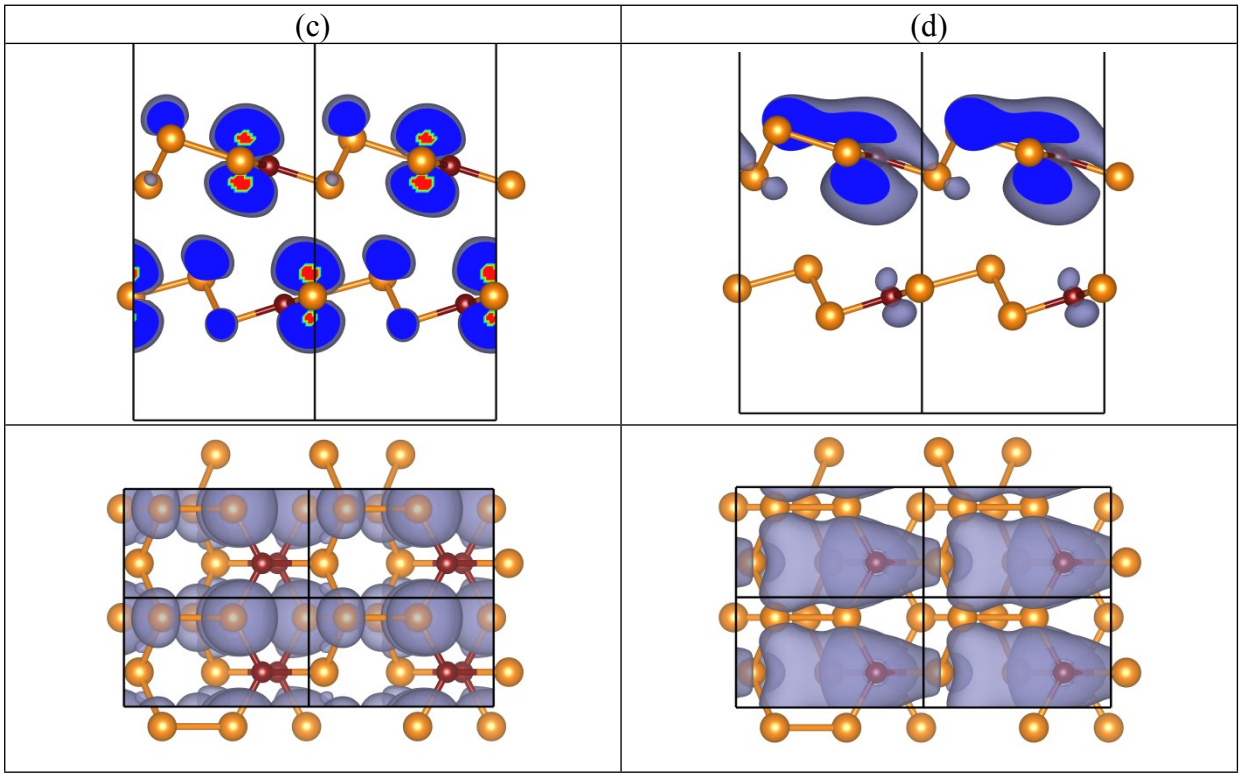


Figure S5. Charge density distributions ($\rho(\mathbf{r})$) in the VBM and CBM of the three patterns of α BP_3 bilayer: AA (a, b), AB'(c, d), and AC (e, f). Two different views are shown for each of them.





(e)	(f)