Electronic Structure Engineering of Various Structural Phases of Phosphorene

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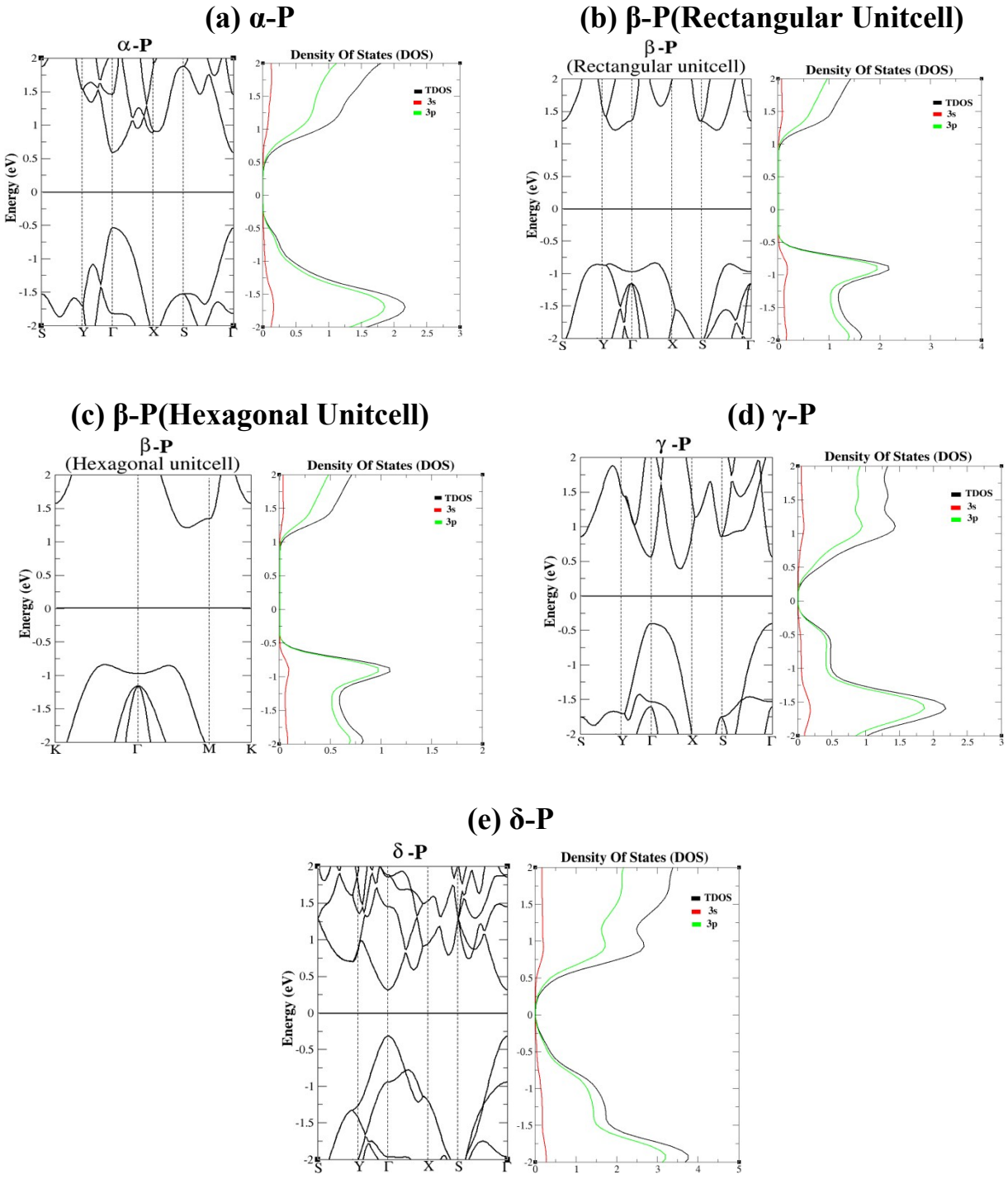

FIGURE S1. The band structure of the pristine (a) α-P, (b) β-P (rectangular unitcell), (c) β-P (hexagonal unitcell) (d) γ-P and (e) δ-P monolayers along with the density of states showing contribution of 3s, 3p orbitals and the total density of states (TDOS).

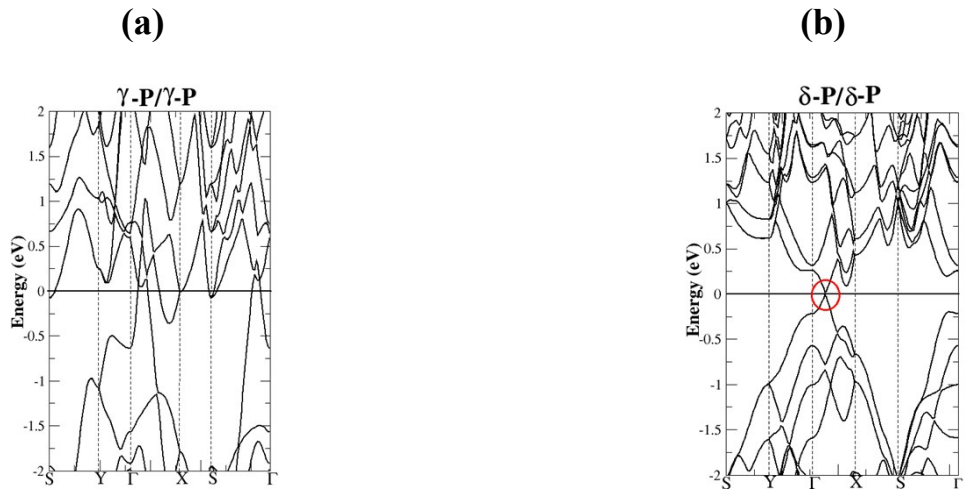

FIGURE S2. The electronic band structure of the homo-bilayers of (a) γ-P and (b) δ-P using GGA-PBE functional. The Dirac cone features in δ-P homo-bilayer is highlited with red circle in (b).

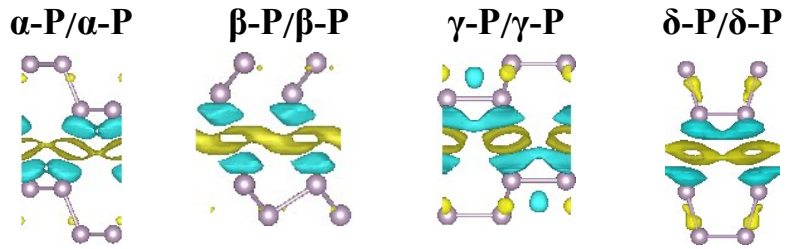

FIGURE S3. The side view of charge density difference profile for homo-bilayers of phosphorene allotropes. Isosurface value is taken as 2.6 x 10^{-4} e/Å^3. Blue and yellow region shows charge depletion and accumulation respectively.

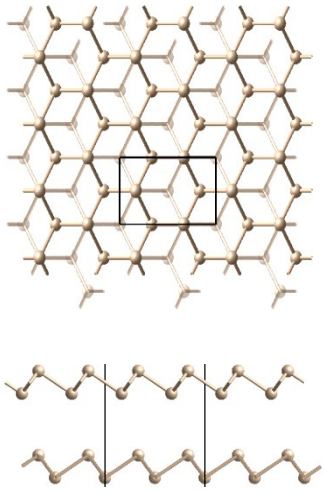

FIGURE S4. The homo-bilayer of AB stacked bilayer of β-P in rectangular unitcell with a= 3.32 Å and b= 5.74 Å with top and side view.

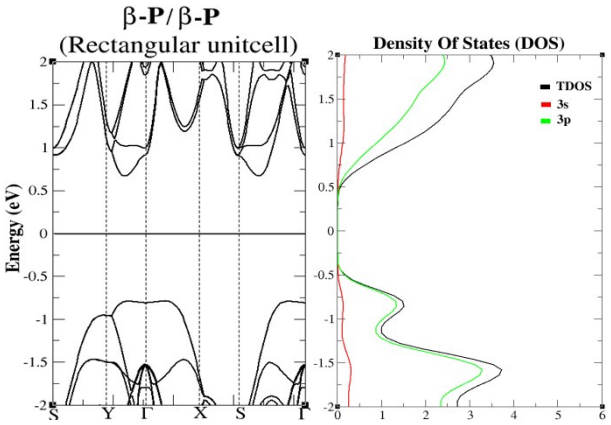

FIGURE S5. The electronic band structure and DOS of bilayer β-phosphoerene in AB-stacked rectangular unit cell.

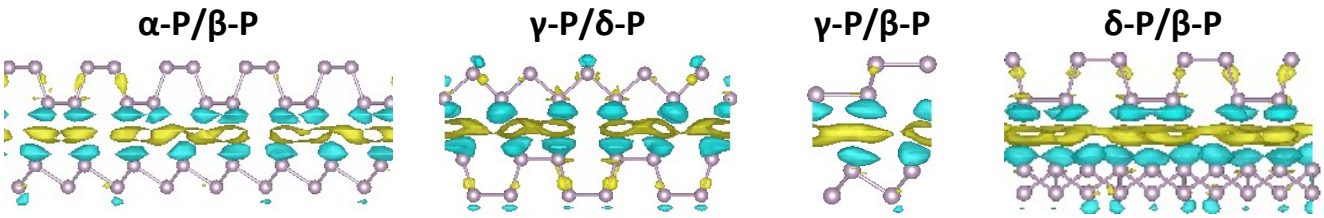

FIGURE S6. The side view of charge density difference profile for hetero-bilayers of phosphorene allotropes. Isosurface value is taken as 2.4 x 10^{-4} e/Å^3. Blue and yellow regions show charge depletion and accumulation respectively.

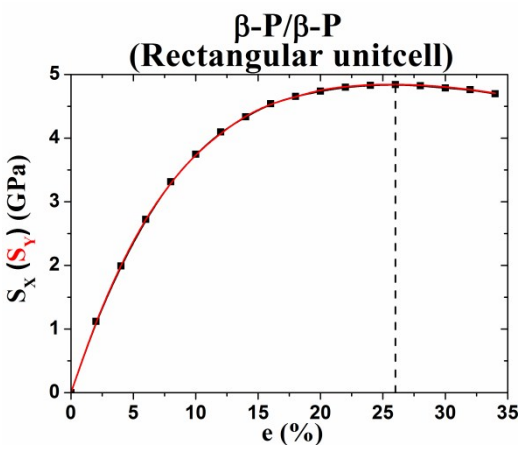

FIGURE S7. Stress-strain curve for β-P bilayer in rectangular unitcell.

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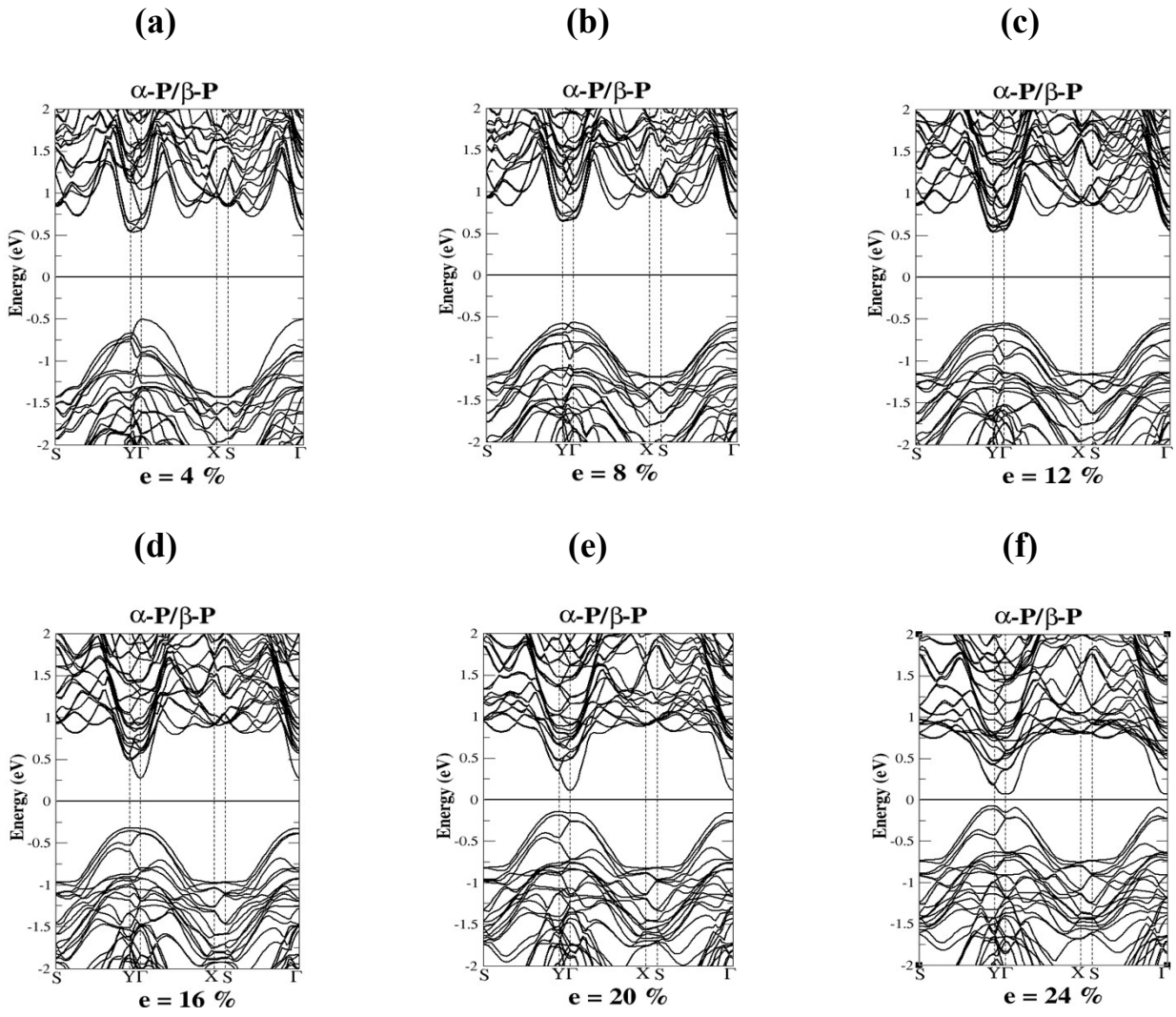

FIGURE S8. The electronic band structure of α-P/β-P at various values of biaxial tensile strain (e).

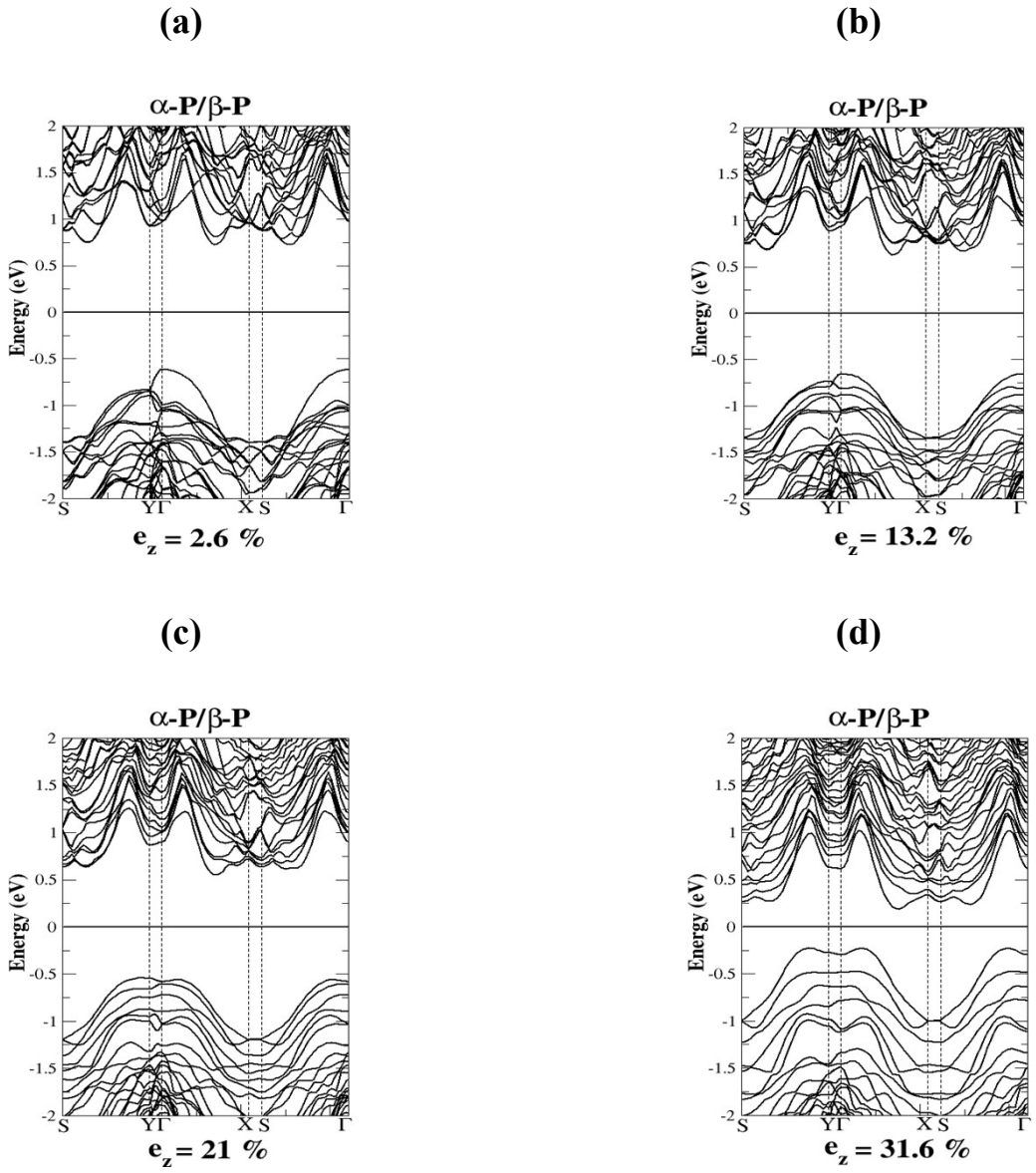

FIGURE S9. The electronic band structure of α-P/β-P at various values of normal compression strain (e_z).

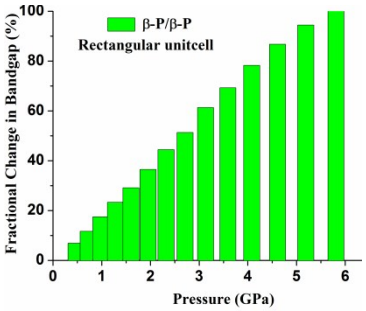

FIGURE S10. The variation of fractional change in bandgap with pressure for β-P bilayer in rectangular unitcell.

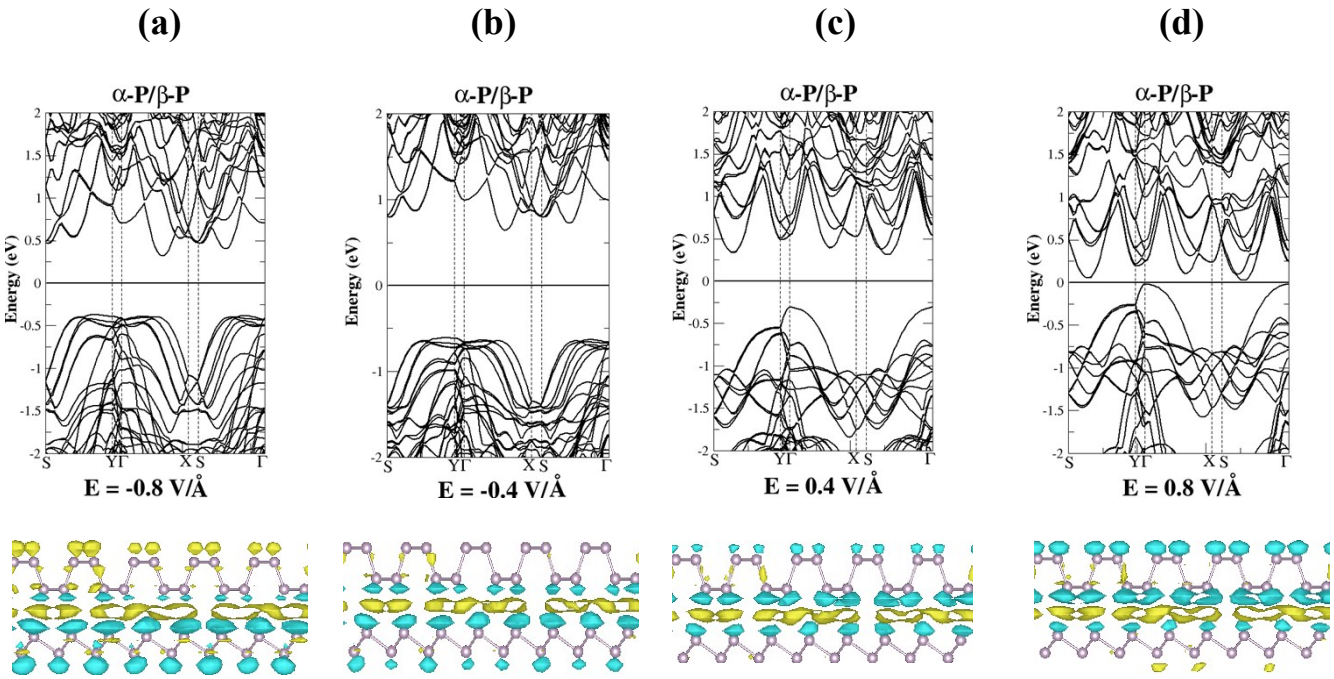

FIGURE S11. The electronic band structures and isosurfaces of charge accumulation and charge depletion of α-P/β-P hetero-bilayer at different values of applied electric field.Blue and yellow region shows charge depletion and accumulation respectively.