Supplementary Information (SI) of "Electric field tunable band-gap crossover in black(blue) phosphorus/g-ZnO van der Walls heterostructures"

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Outline

SI.1: Convergence tests.

black-p/g-ZnO

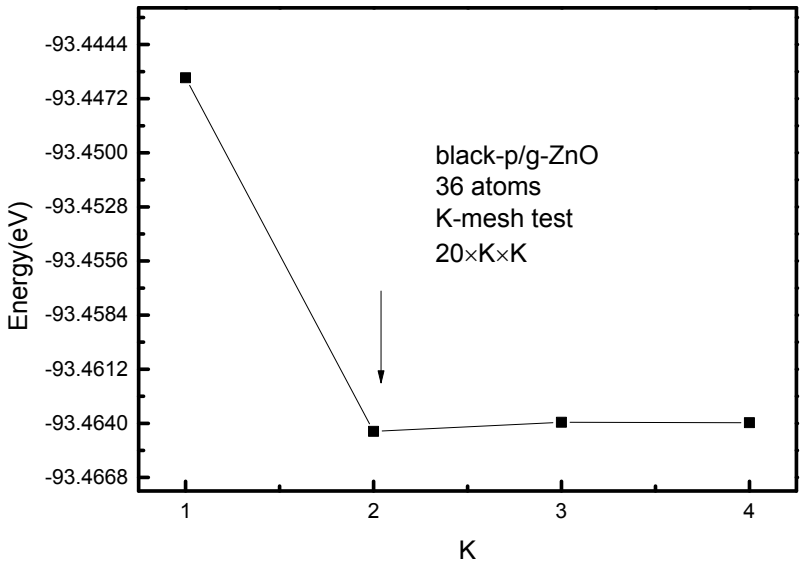


Fig. S1.1 Change of energy of black-p/g-ZnO with k-point meshes (20×K×K).

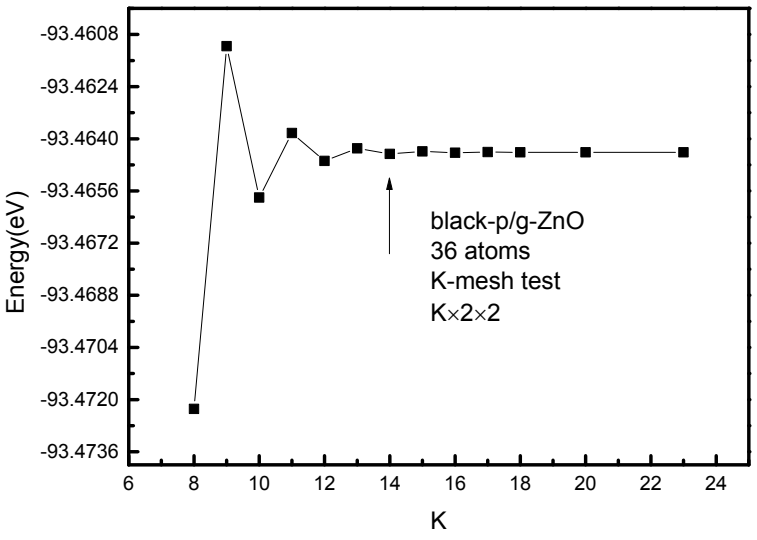


Fig. S1.2 Change of energy of black-p/g-ZnO with k-point meshes (K×2×2).

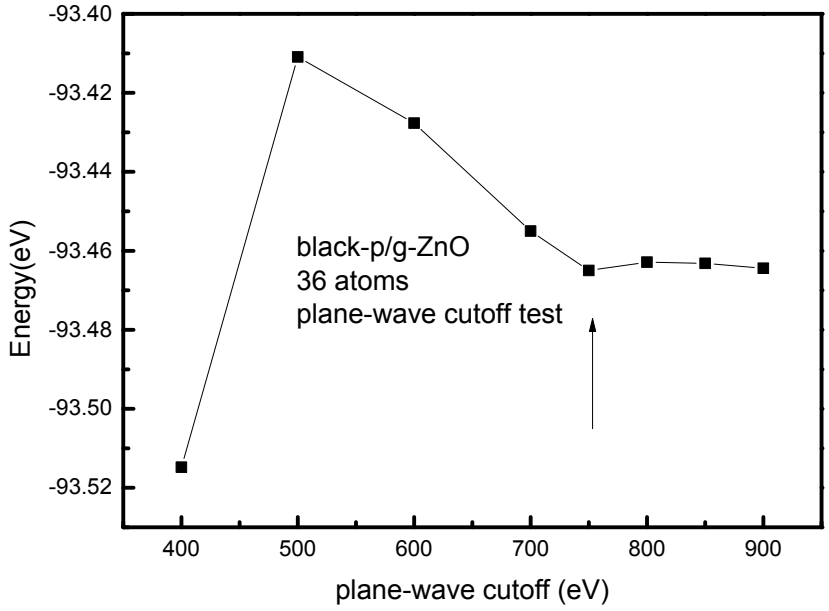


Fig. S1.3 Change of energy of black-p/g-ZnO with plane-wave cutoffs.

blue-p/g-ZnO

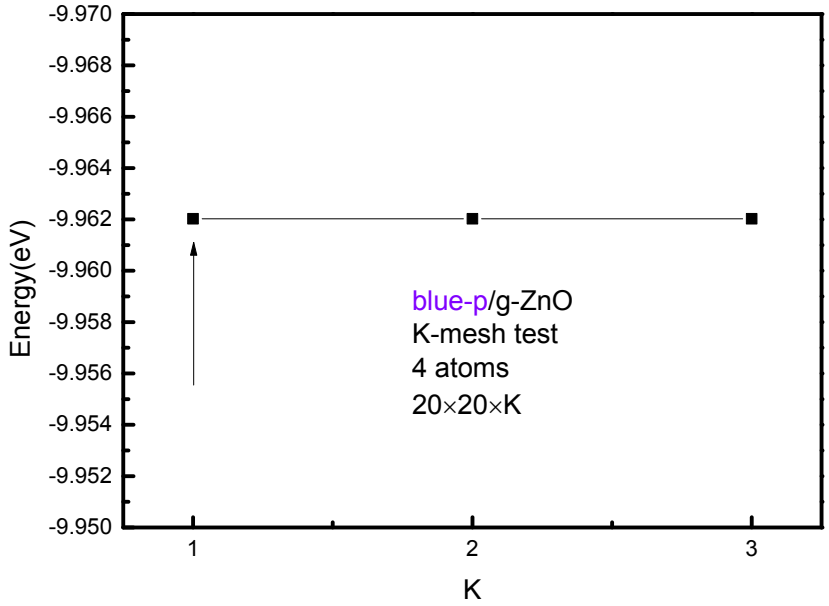


Fig. S1.4 Change of energy of blue-p/g-ZnO with k-point meshes (20×20×K).

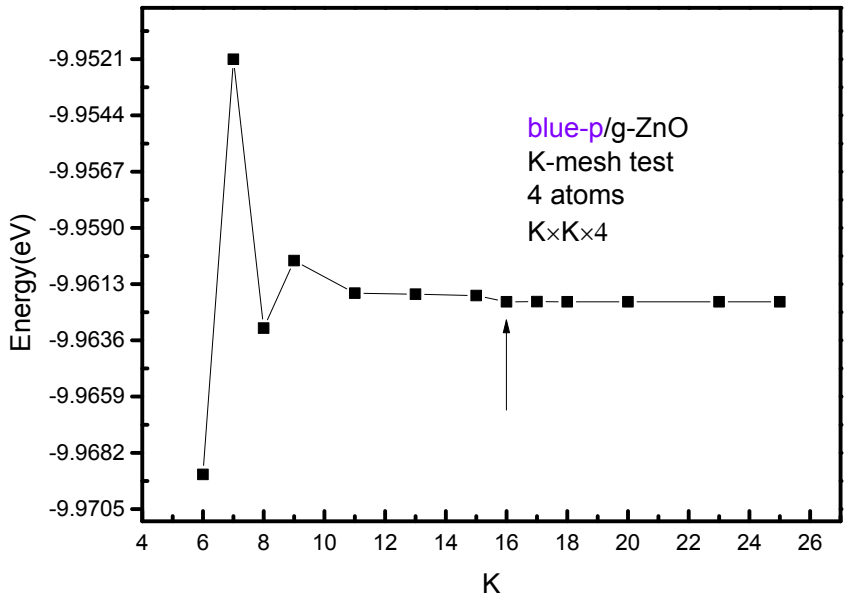


Fig. S1.5 Change of energy of blue-p/g-ZnO with k-point meshes (K×K×4).

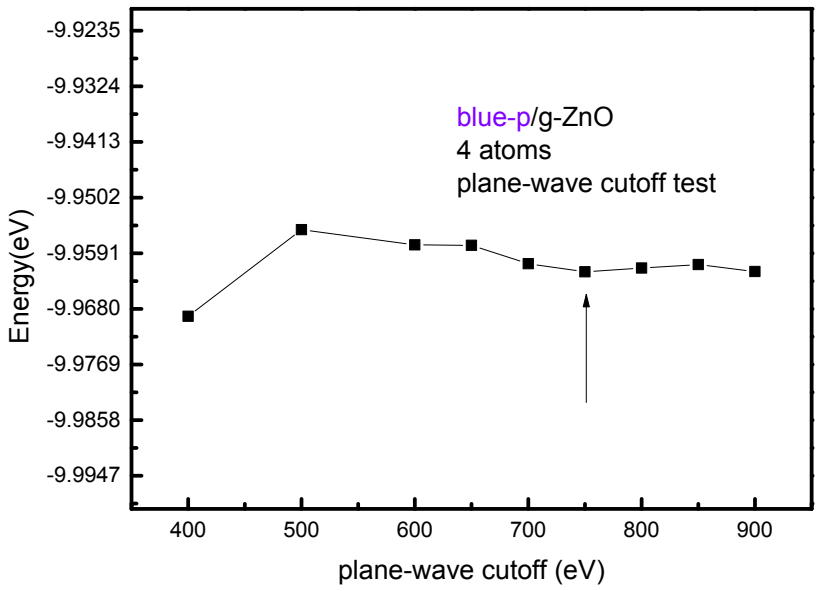
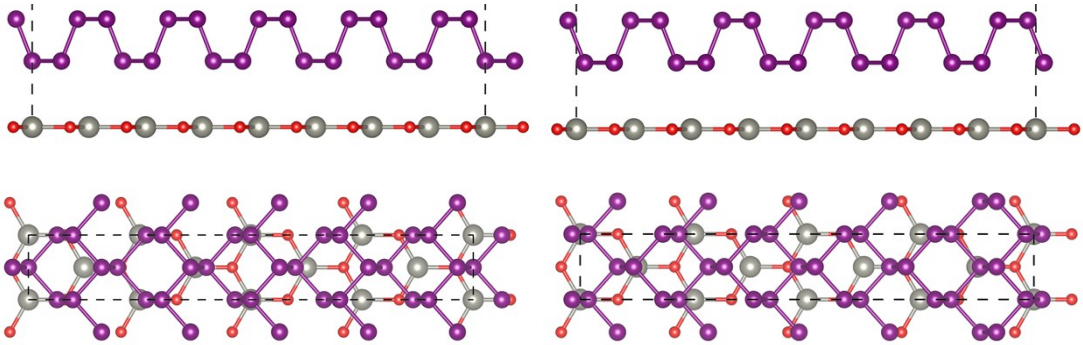


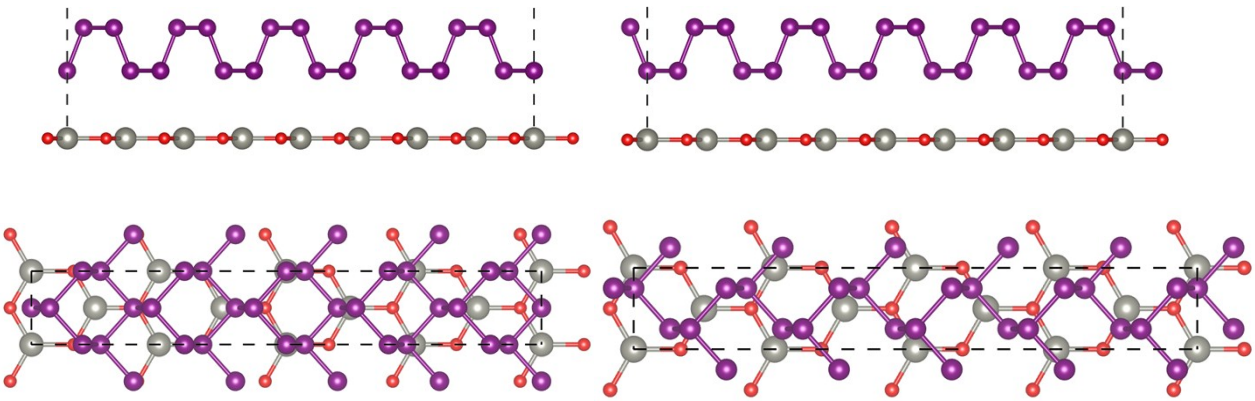
Fig. S1.6 Change of energy of blue-p/g-ZnO with plane-wave cutoffs.

SI.2: Other typical patterns of heterostructures.

black-p/g-ZnO



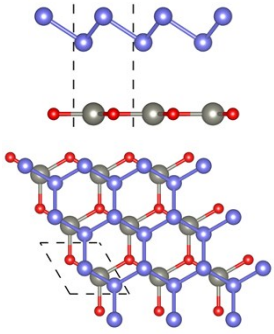
I ΔE=0 II ΔE=29.94 meV



III ΔE=33 meV IV ΔE=76.31 meV

Fig. S2.1 Relative energy of other typical patterns of black-p/g-ZnO.

blue-p/g-ZnO



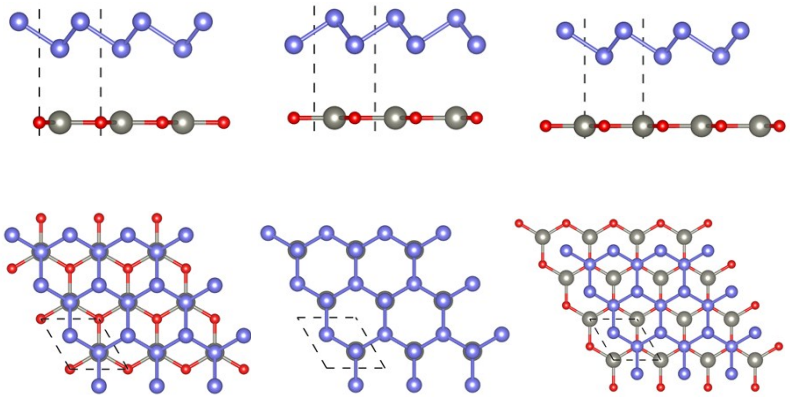
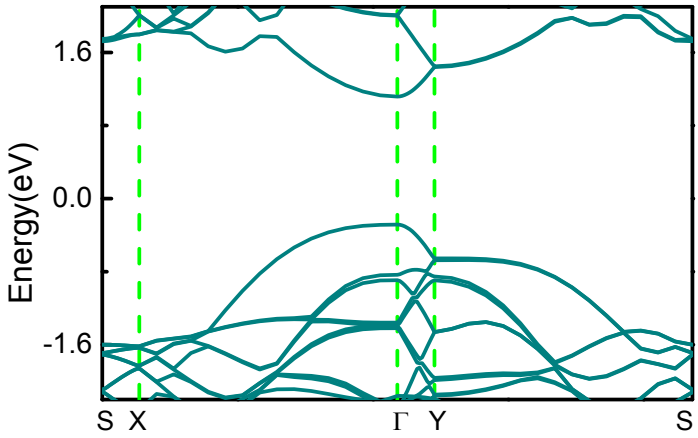


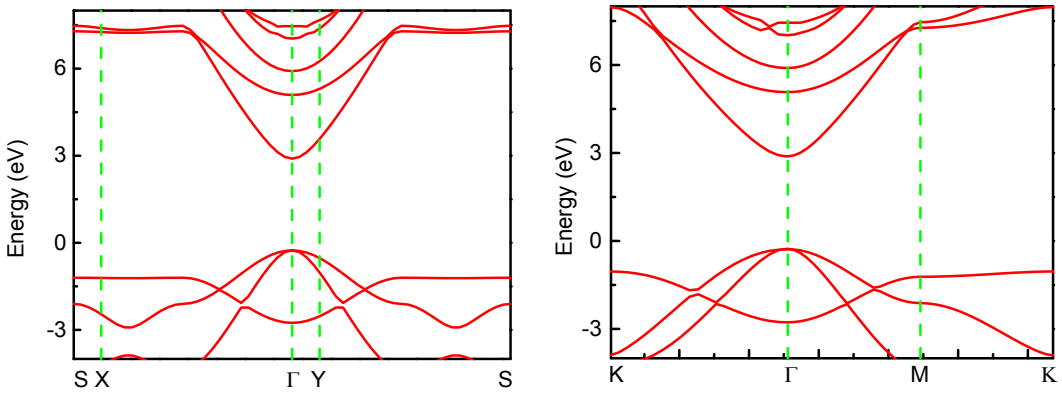
Fig. S2.2 Relative energy of other typical patterns of blue-p/g-ZnO.

SI.3: Band structures of isolated black-p, g-ZnO and blue-p.



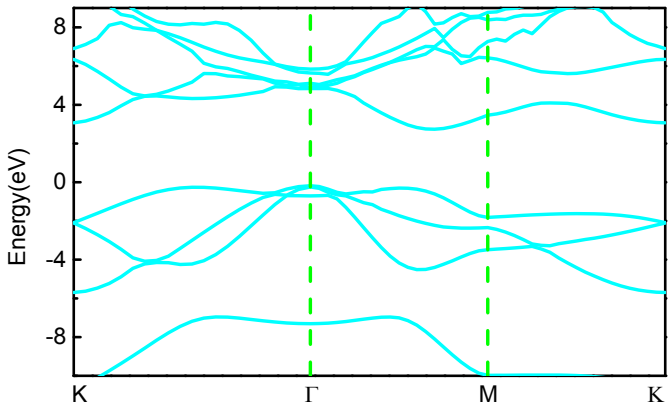
isolated black-p E_g=1.38 eV

Fig. S3.1 Band structures of isolated black-p.



isolated g-ZnO E_g=3.29 eV

Fig. S3.2 Band structures of isolated g-ZnO.



isolated blue-p E_g=2.86 eV

Fig. S3.3 Band structures of isolated blue-p.

SI.4: Calculations of differential charge density.

$\rho(x,y,z)$

$\Delta\rho(z)$ without E

$\Delta\rho(z)=\int\rho$(blue-p/g-ZnO)$dxdy$-$\int\rho$(blue-p) $dxdy$ -$\int\rho$(g-ZnO) $dxdy$ **(Eq. S4.1)**

ρ(blue-p) and ρ(g-ZnO) are the charge density of blue-p and g-ZnO single-layer in the supercell of heterostructure, respectively. (x,y,z) denote the positions in the supercell.

$\Delta\rho_E(z)$ with E

$\Delta\rho_E(z)= \int\rho_E$(blue-p/g-ZnO)$dxdy$-$\int\rho$(blue-p/g-ZnO)$dxdy$ **(Eq. S4.2)**

ρ_E(blue-p/g-ZnO) and ρ(blue-p/g-ZnO) are the charge density of blue-p/g-ZnO with and without E.

SI.5: Evolution of band-gap of blue-p/g-ZnO with E.

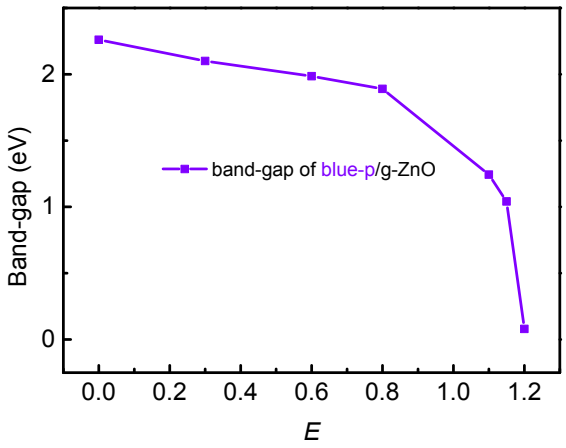


Fig. S5. Evolution of band-gap of blue-p/g-ZnO with E.