

Supplementary Materials

ShuangYing Ma,[†] Chaoyu He,[†] L. Z. Sun,^{*,‡} Haiping Lin,[¶] Youyong Li,[¶] and K.
W. Zhang^{*,†}

*School of Physics and Optoelectronics, Xiangtan University, Xiangtan 411105, China,
Hunan Provincial Key laboratory of Thin Film Materials and Devices, School of Material
Sciences and Engineering, Xiangtan University, Xiangtan 411105, China, and Institute of
Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou 215123, China*

E-mail: lzsun@xtu.edu.cn; kwzhang@xtu.edu.cn

*To whom correspondence should be addressed

[†]School of Physics and Optoelectronics, Xiangtan University, Xiangtan 411105, China

[‡]Hunan Provincial Key laboratory of Thin Film Materials and Devices, School of Material Sciences and Engineering, Xiangtan University, Xiangtan 411105, China

[¶]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou 215123, China

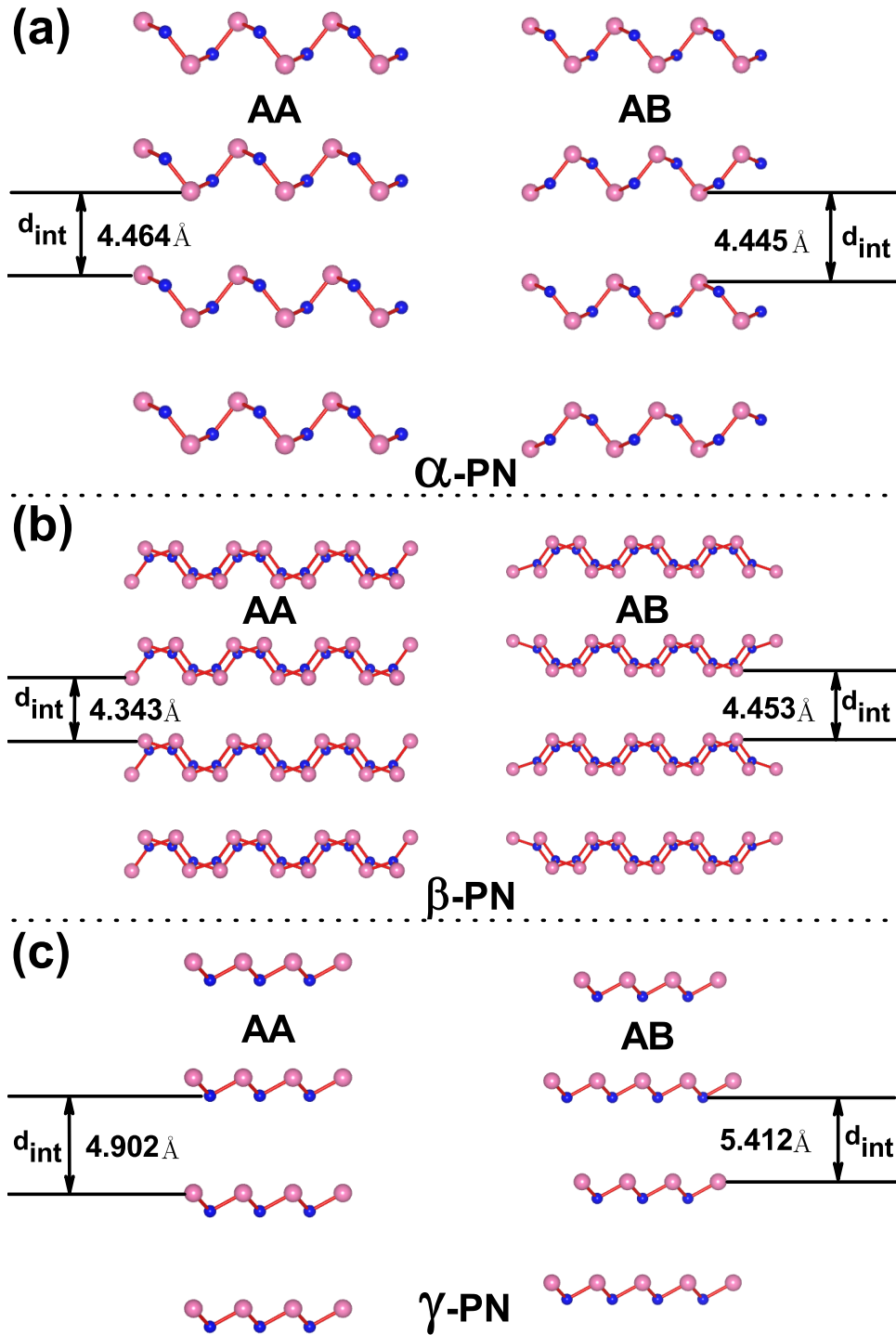


Figure 1: (a), (b) and (c) respectively stands for 3x3 supercell of the well-optimized side elevation of 4 layer α , β and γ -PN. The balls in blue and pink represent nitrogen and phosphorus atoms respectively. AA and AB stand for two kinds of stacking orders. d_{int} stand for side interlayer spacing of the three phases.

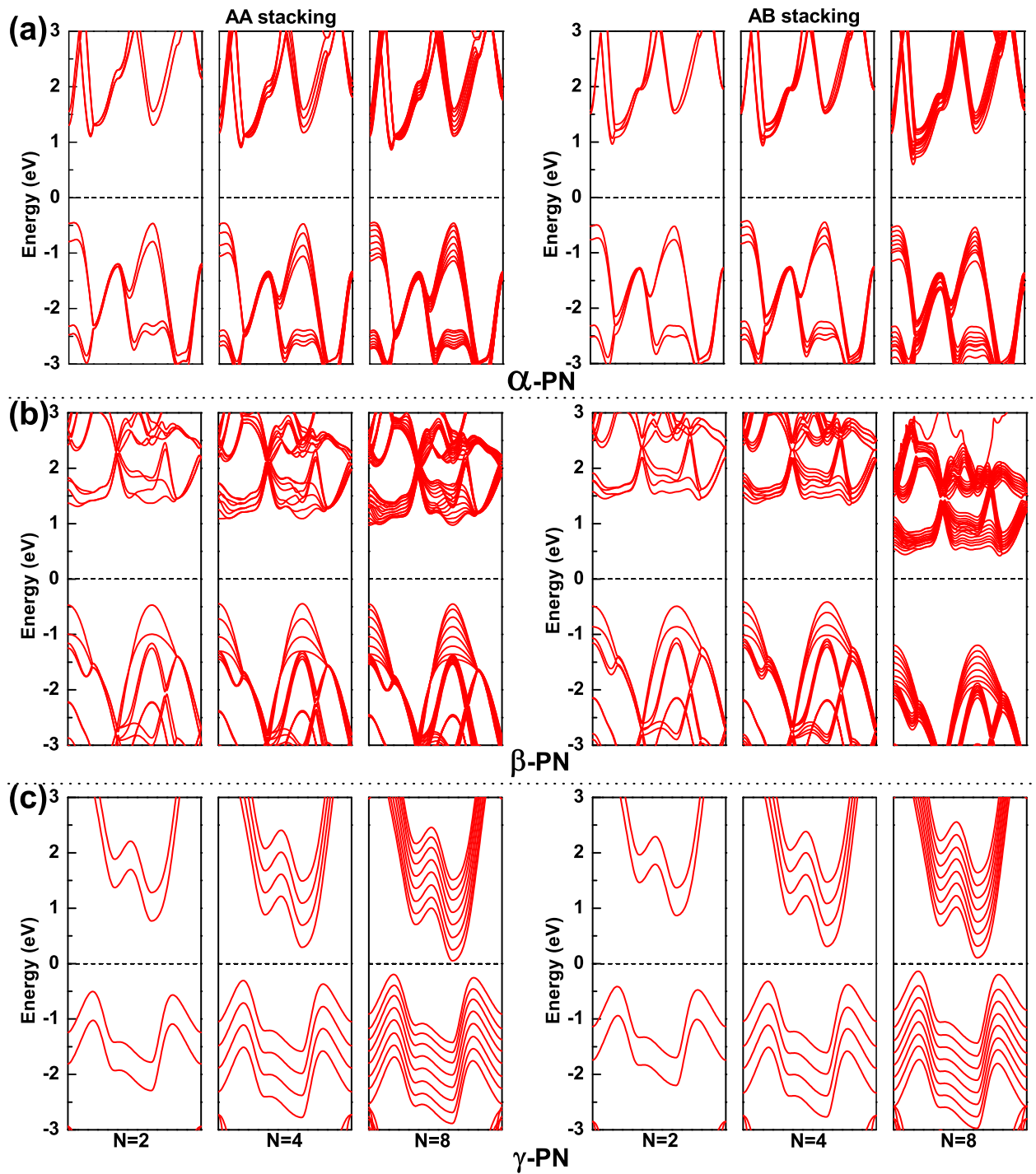


Figure 2: (a), (b) and (c) respectively stands for thickness-dependence of the band gap for α , β and γ phase. The letter M stands for the number of layers.

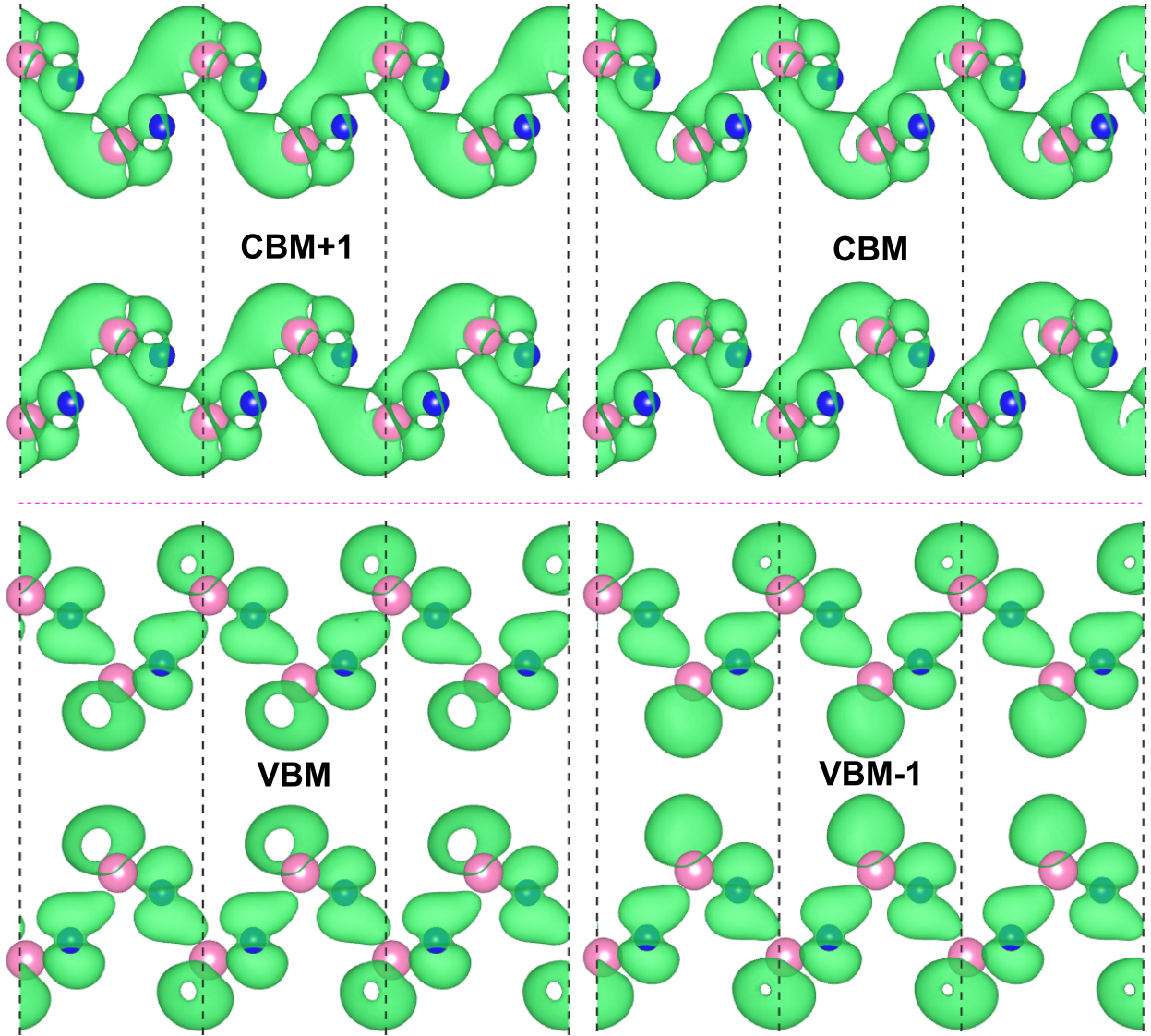
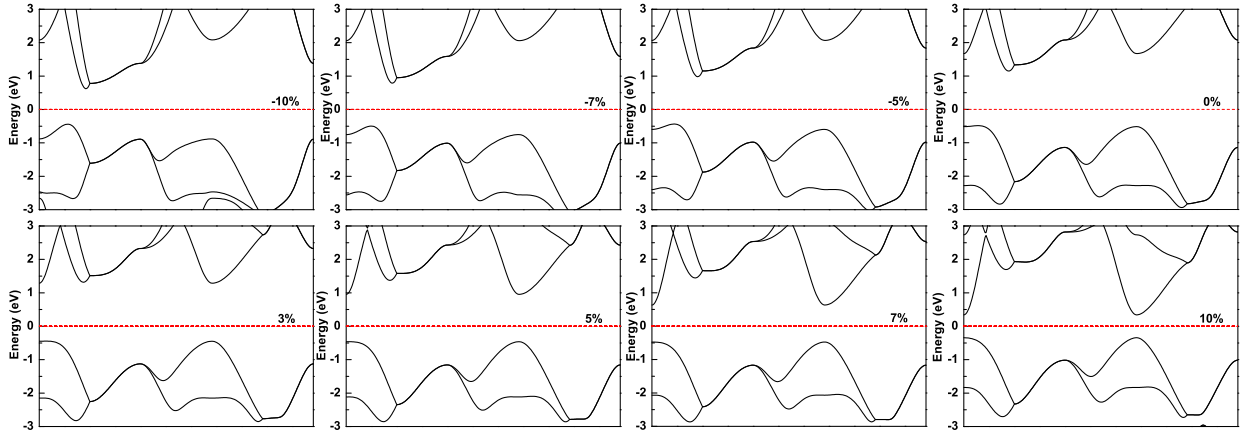


Figure 3: The charge density of the valence band maximum (VBM), VBM-1, conduction band bottom (CBM), CBM+1 for two layered α -PN with AA stacking. The isosurface is $0.003 \text{ e}/\text{\AA}^3$. “-1” and “+1” respectively stands for down and up one energy level.

(a) band structure with strain for α phase along lattice vector a



(b) band structure with strain for α phase along lattice vector b

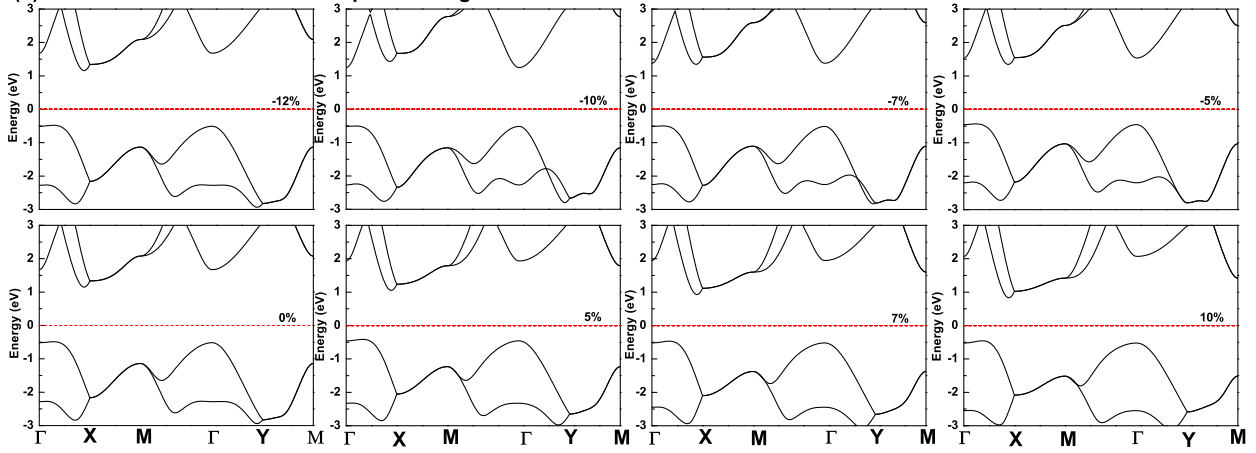
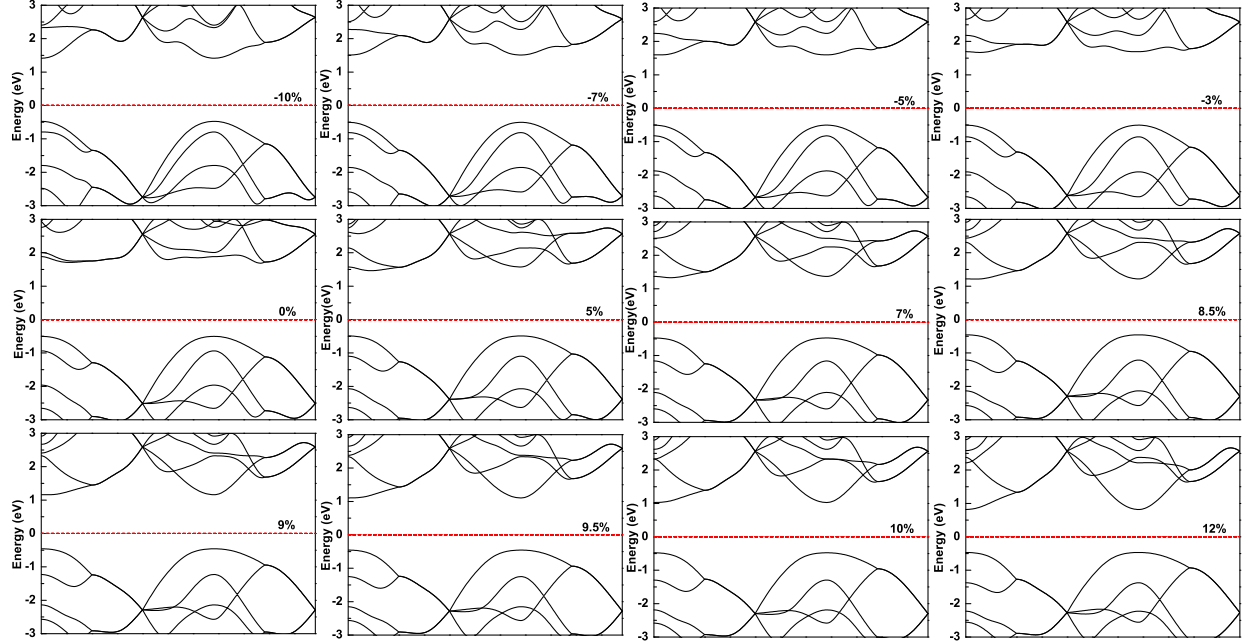


Figure 4: (a) and (b) show the band gap as a function of strain for α -PN.

(a) band structure with strain for β phase along lattice vector b



(b) band structure with strain for β phase along lattice vector a

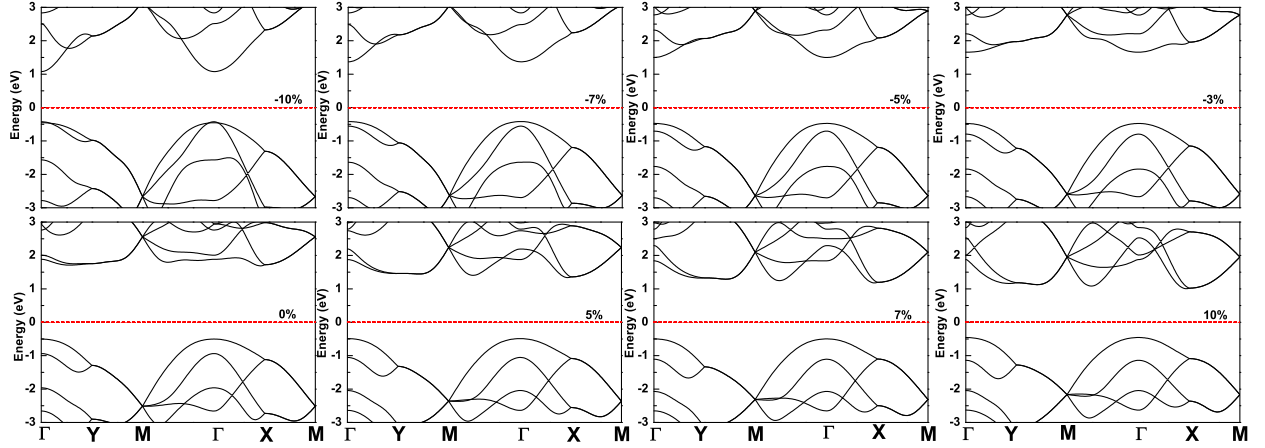


Figure 5: (a) and (b) show the band gap as a function of strain for β -PN.