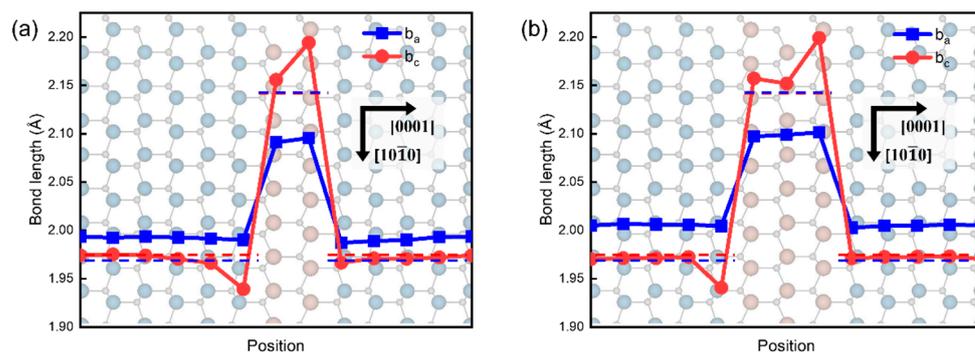
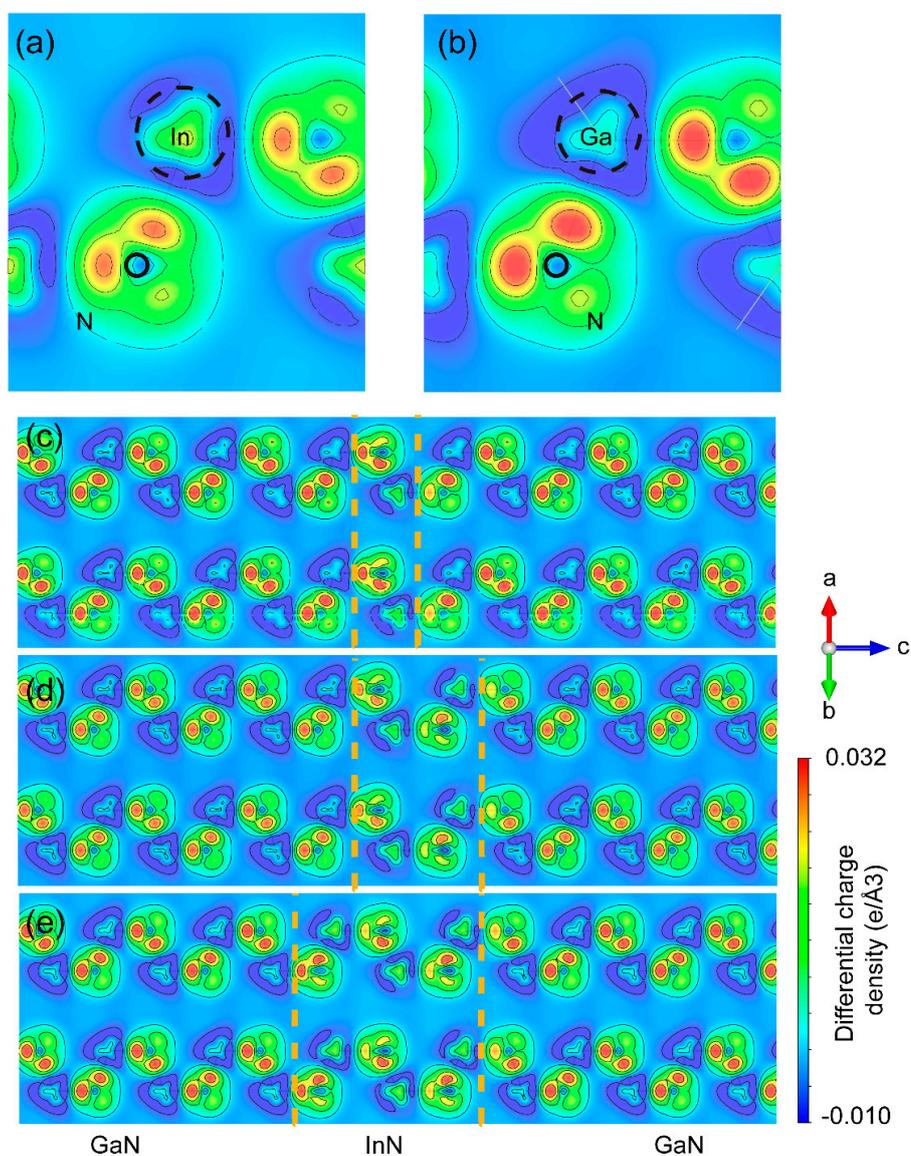


# Supplementary Material

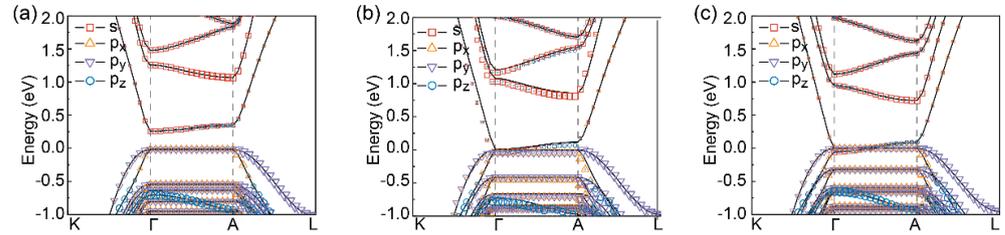


**Figure S1** (a), and (b) were the distributions of bond lengths  $b_a$  and  $b_c$  along the direction  $[0001]$  in  $\text{InN}_2/\text{GaN}_{10}$ , and  $\text{InN}_3/\text{GaN}_9$  respectively. The atomic crystal structures were the side view of the periodic extended  $\text{InN}_2/\text{GaN}_{10}$ , and  $\text{InN}_3/\text{GaN}_9$  respectively.

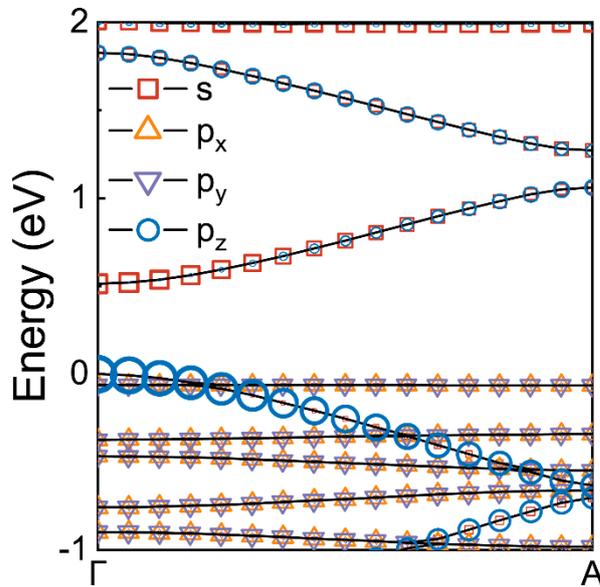


**Figure S2** Differential charge densities of InN, GaN, and InN/GaN SL. (a) and (b) were the contour plots of the differential charge densities in a  $(11\bar{2}0)$  slice of InN and GaN respectively. (c), (d) and

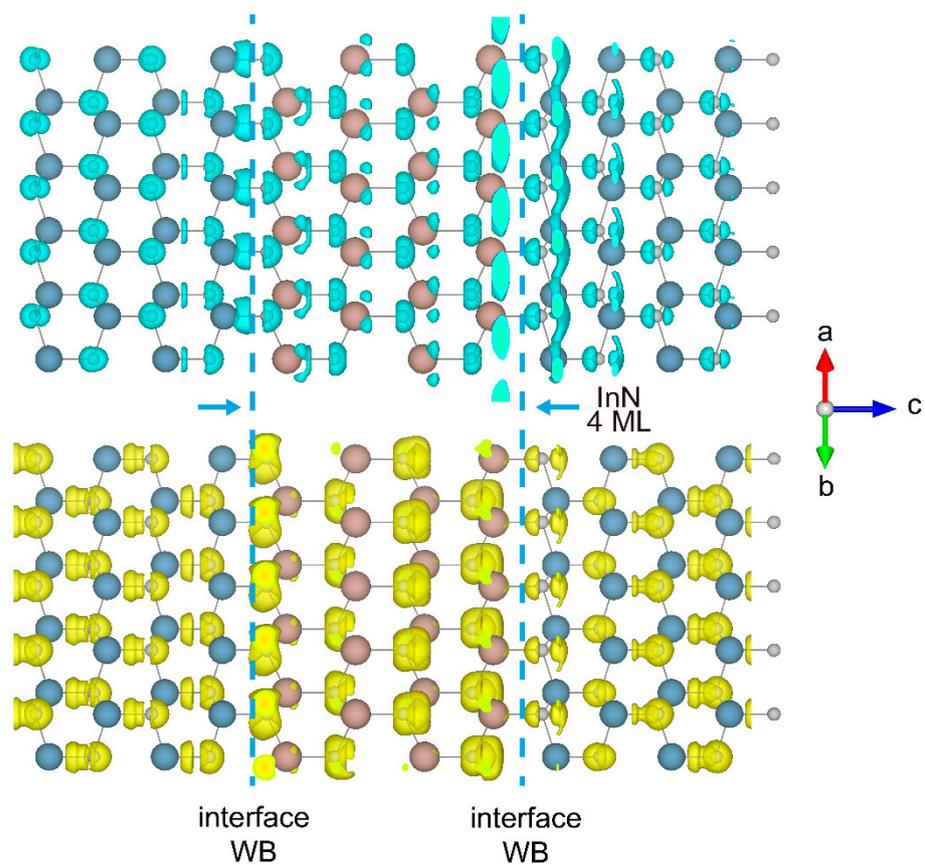
(e) were the contour plots of the differential charge densities in a  $(11\bar{2}0)$  slice of  $\text{InN}_1/\text{GaN}_{11}$ ,  $\text{InN}_2/\text{GaN}_{10}$  and  $\text{InN}_3/\text{GaN}_9$  respectively. The InN and GaN areas were divided by the yellow dashed lines. The compass and the axis labels were used to calibrate the orientation of the lattice. The different colors were used to represent the positive and negative values of differential charge densities.



**Figure S3** (a), (b) and (c) shown band structures between K and L points of  $\text{InN}_2/\text{GaN}_{10}$ ,  $\text{InN}_3/\text{GaN}_9$  and  $\text{InN}_4/\text{GaN}_8$ , respectively.



**Figure S4** The electronic band structure of  $\text{InN}_1/\text{GaN}_7$  under 8% tensile strain.



**Figure S5** Distributions of injected electrons and holes. Blue and yellow surfaces represented contour planes of electrons and holes with charge density of  $0.01 e/\text{\AA}^3$ . The InN and GaN areas were divided by the blue dashed lines.