Supporting Information for

Strain-tunable optoelectronic and photocatalytic properties of 2D GaN/$MoSi_2P_4$ heterobilayers: Potential optoelectronic/photocatalytic materials

Huabing Shu[*a], Feifan Wang[b], Kai Ren[*c], Jiyuan Guo[a]

[a] *School of Science, Jiangsu University of Science and Technology, Zhenjiang 212001, China*

[b] *Jiangsu Co-Innovation Centre of Efficient Processing and Utilization of Forest Resources, College of Chemical Engineering, Nanjing Forestry University, Nanjing 210037, China*

[c] *School of Mechanical and Electronic Engineering, Nanjing Forestry University, Nanjing 210037, China*

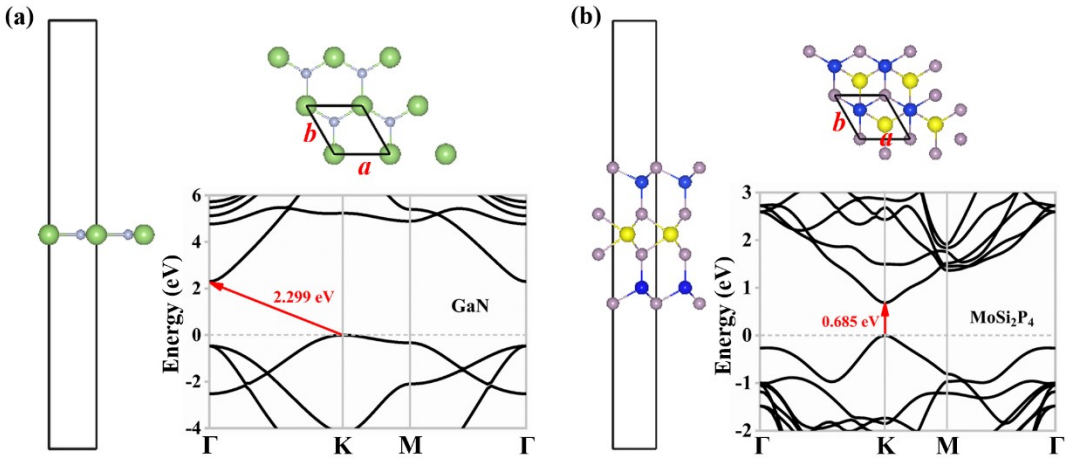

Fig. S1 Top (side) views and band structures of isolated monolayers: (a) GaN and (b) $MoSi_2P_4$. The band structures are calculated by the PBE method.

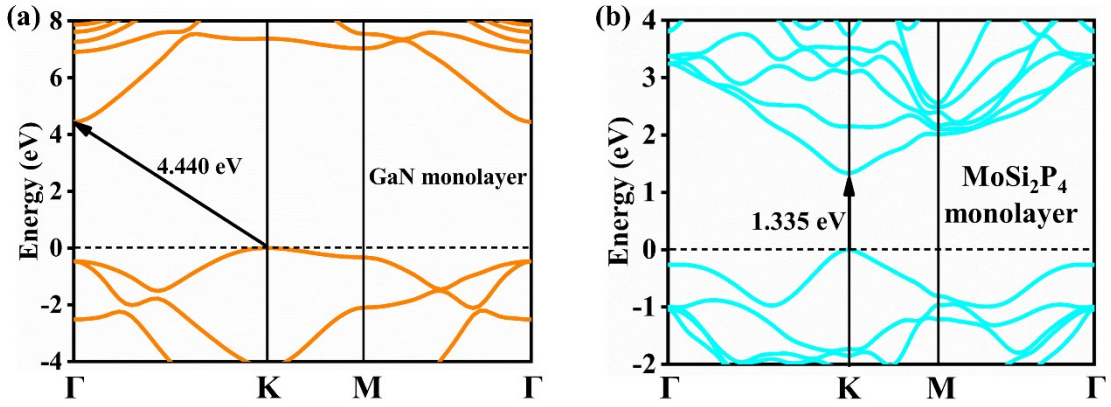

Fig. S2 Quasi-particle band structures of GaN monolayer and $MoSi_2P_4$ monolayer at G_0W_0 level.

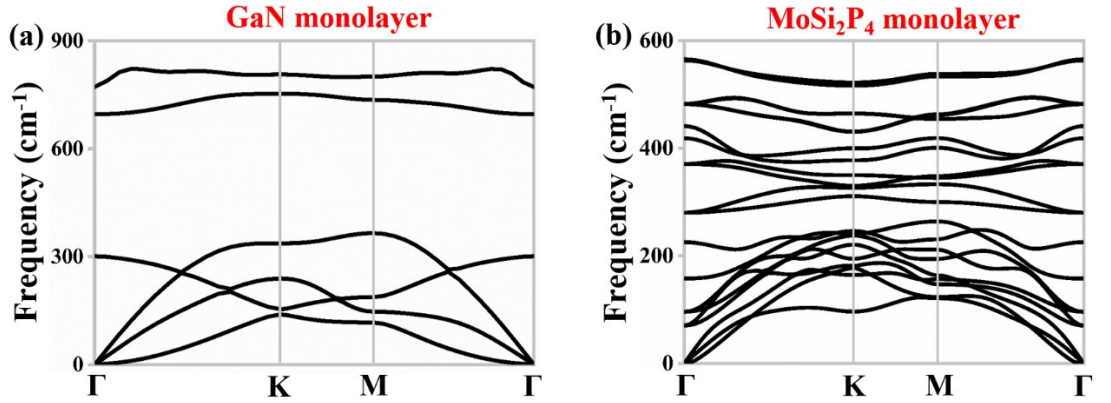

Fig. S3 Phonon spectra of isolated GaN and $MoSi_2P_4$ monolayers.

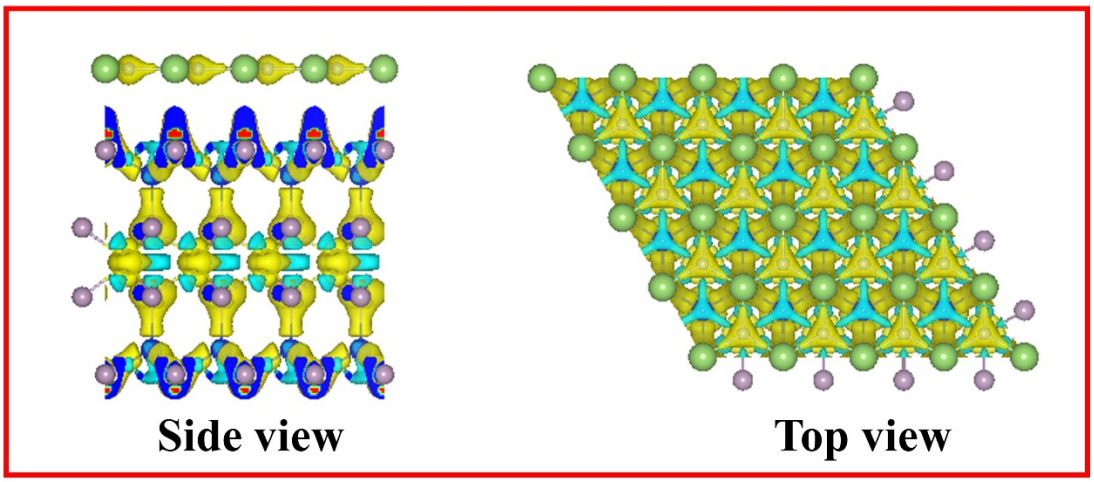

Fig. S4 Differential charge density with an isosurface value of 1.0×10^{-3} e·Å^{-3} along the ***c*** direction for the AA5 GaN/$MoSi_2P_4$ heterosbilayer. The yellow and cyan suggest the gain and loss of electrons, respectively.

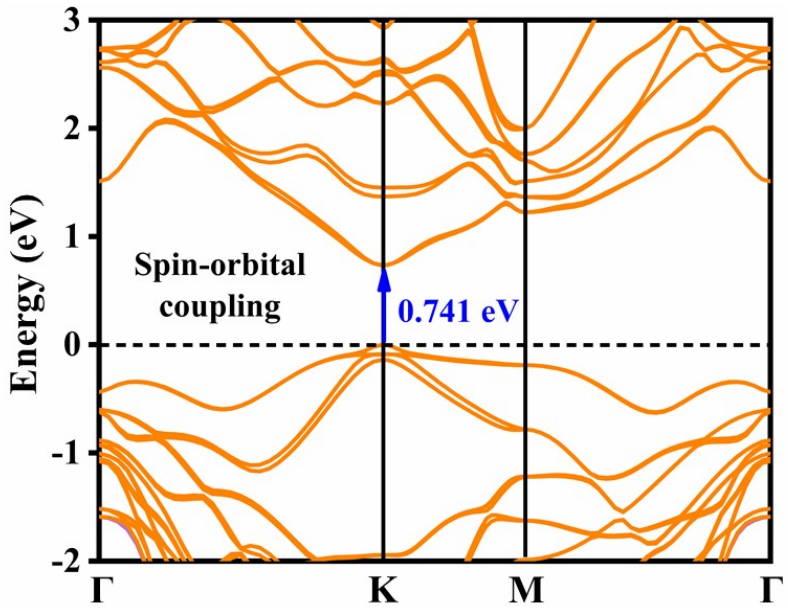

Fig. S5 Calculated band structures of the AA5 GaN/$MoSi_2P_4$ heterobilayer with the spin-orbit coupling effects at the PBE level.

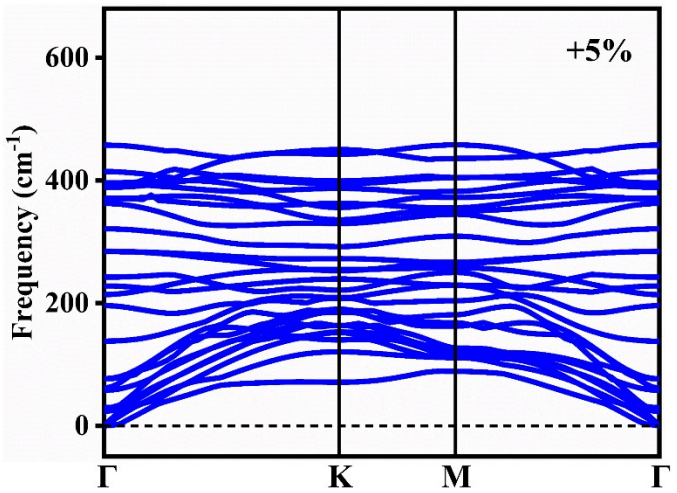

Fig. S6 Phonon spectrum of AA5 GaN/$MoSi_2P_4$ heterosbilayer at +5% biaxial tensile strain.

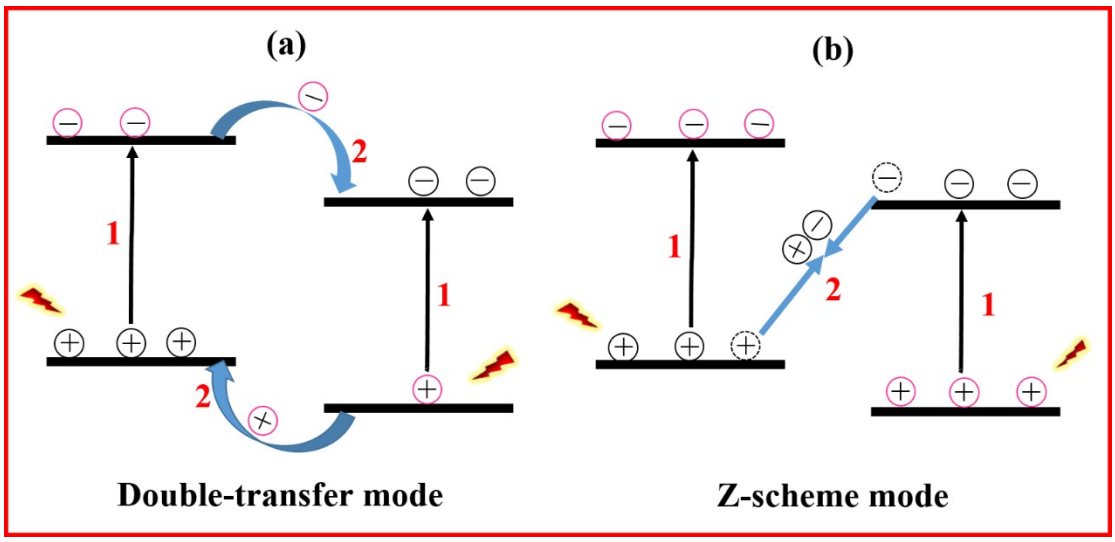

Fig. S7 Two kinds of modes of charge transfer in type-II heterostructure: (a) Double-transfer mode, (b) Z-scheme mode.

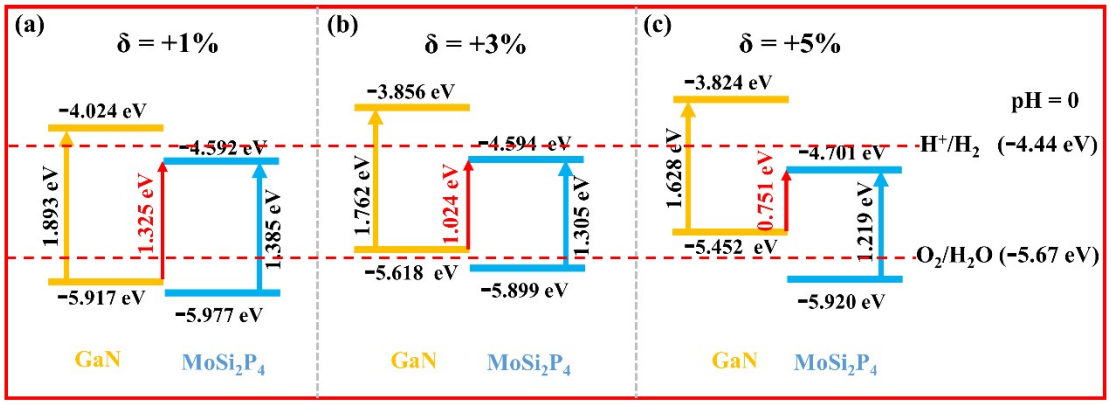

Fig. S8 The positions of two band edges of $GaN/MoSi_2P_4$ vdW heterostructure compared to the vacuum level under different tensile strains: (a) +1%, (b) +3%, (c) +5%. The calculated results are based on the G_0W_0 level.