Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Appendix A. Supplementary data

Fig.S1 The refined partial density of state of GaN/C_2N heterostructure.

Fig.S2 The refined partial density of states of GaN/C_2N+2P heterostructure.

Fig.S3 The projected band diagrams of GaN/C_2N heterostructure doped with (a) one P atom, (b) one As atom, and (c) two As atoms using the HSE06 method.

Fig.S4 The optical absorption spectra of all doped GaN/C_2N heterostructures, as well as the pristine monolayers of GaN and C_2N, calculated using the HSE06 method.

Fig.S5 The (a) real and (b) imaginary parts of the dielectric function of all doped GaN/C_2N heterostructures, as well as the pristine monolayers of GaN and C_2N, calculated using the HSE06 method.

Fig.S6 The (a) reflectivity and (b) refractive index of all doped GaN/C_2N heterostructures, as well as the pristine monolayers of GaN and C_2N, calculated using the HSE06 method.

Fig.S7 The projected band diagrams of GaN/C_2N heterostructure with different compressive strains (a) -1%, (b) -2%, and (c) -3% calculated using the HSE06 method.

Fig.S8 The projected band diagrams of GaN/C_2N heterostructure with different tensile strains (a) 1%, (b) 2%, and (c) 3% calculated using the HSE06 method.

Fig.S9 The influence of strain on the absorption spectrum of GaN/C_2N heterostructure, calculated using the HSE06 method.

Fig.S10 The (a) real and (b) imaginary parts of the dielectric function of GaN/C_2N heterostructures with different strains, calculated using the HSE06 method.

Fig.S11 The reflectivity (a) and refractive index (b) of GaN/C_2N heterostructures with different strains, calculated using the HSE06 method.