Electronic Supplementary Material (ESI) for RSC Advances.


# Electronic supplementary information

# Theoretical studies on the form and effect of N-doping in $ZnGa_2O_4$ photocatalyst

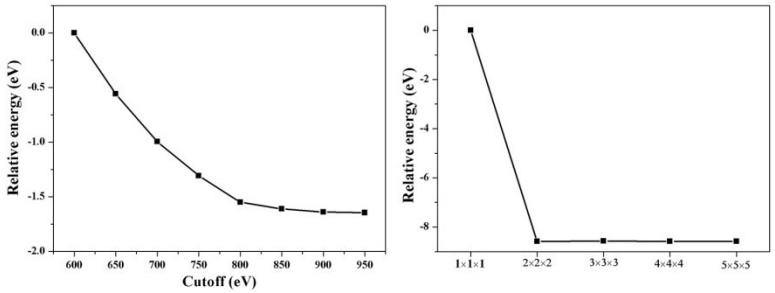


Figure S1. The convergence tests for cutoff and kpoints before theoretical calculations.

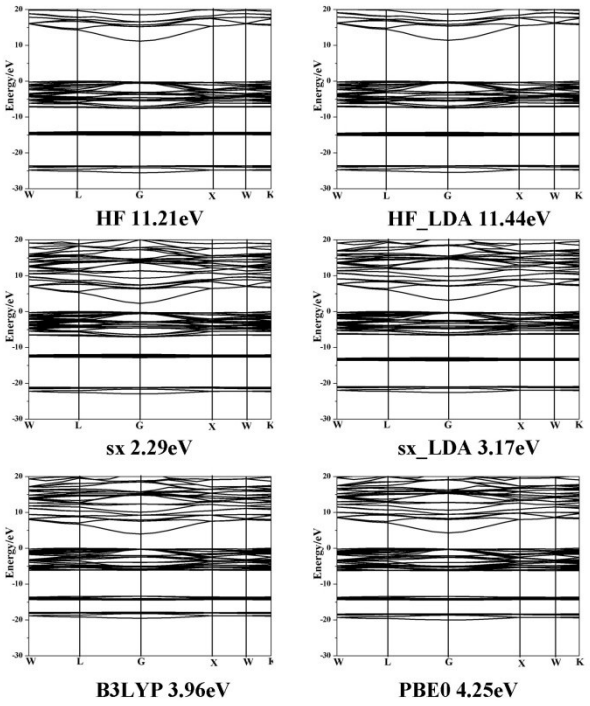


Figure S2. The band structures of $ZnGa_2O_4$ calculated by HF, HF_LDA, sx (screened exchange functional), sx_LDA, B3LYP, and PBE0.

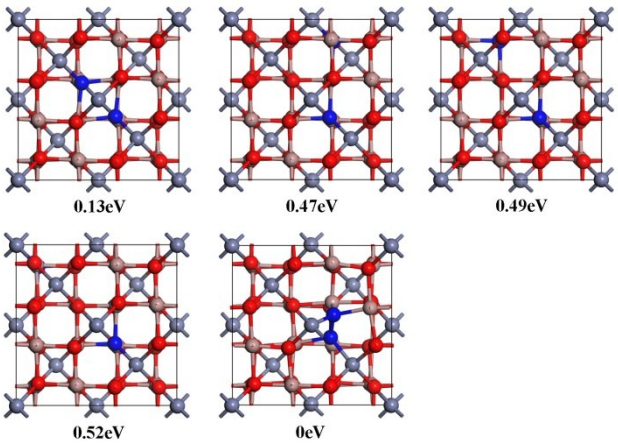


Figure S3. The structures and the relative energies of $2N_s$-doped $ZnGa_2O_4$ with different doping sites.

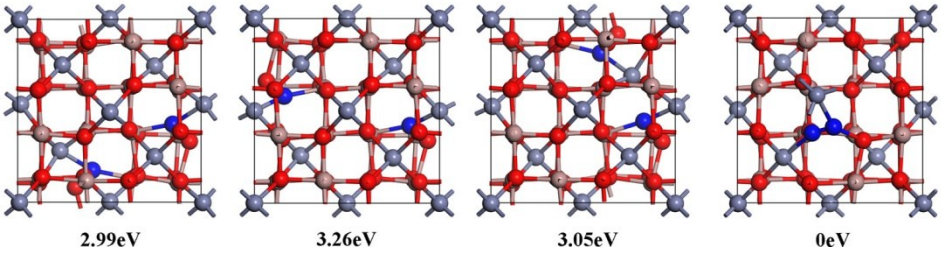


Figure S4. The structures and the relative energies of $2N_i$-doped $ZnGa_2O_4$ with different doping sites.

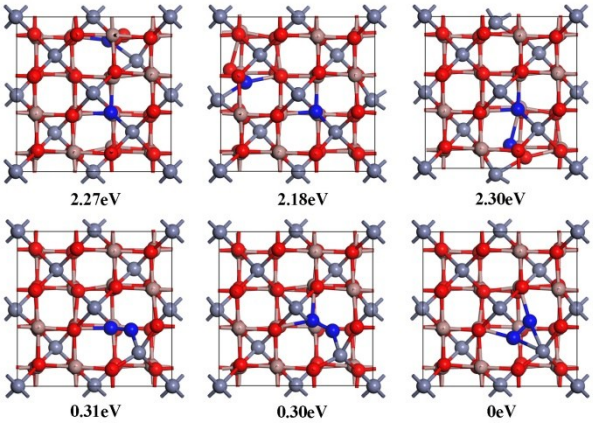


Figure S5. The structures and the relative energies of $N_s$+$N_i$-doped $ZnGa_2O_4$ with different doping sites.