Electronic supplementary information

Theoretical studies on the form and effect of N-doping in ZnGa$_2$O$_4$ photocatalyst

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

Figure S2. The band structures of ZnGa$_2$O$_4$ 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$_2$O$_4$ with different doping sites.

Figure S4. The structures and the relative energies of 2N$_i$-doped ZnGa$_2$O$_4$ with different doping sites.

Figure S5. The structures and the relative energies of N$_s$+N$_i$-doped ZnGa$_2$O$_4$ with different doping sites.