# Supplementary Material

## $g\text{-}C_3N_4$ modified BiOCl visible light catalyst and the enhanced photocatalytic degradation/sterilization performance

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## Computational methods

Within the framework of density functional theory (DFT), the atomic correlation pseudopotential is solved by employing the generalized gradient approximation Perdew-Burke-Ernzerhof (GGA-PBE). Total energy calculation, structural optimization, and photoelectric performance calculation for these structures are obtained via the Vienna *Ab Initio* Simulation Package (VASP). The balance between accuracy and efficiency achieved by VASP is widely acknowledged. More accurate band structures (BS) and density of states (DOS) are attained via the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional. It can avert the band gap error caused by traditional methods (generated by GGA or LDA) and is widely accepted. The electron-electron correlation is described by employing the projector augmented wave (PAW) method. For achieving precise optimizations, a plane-wave basis set with an energy cutoff value between 400 and 500 eV was utilized and k-point grids were generated using the Γ-centered Monkhorst-Pack scheme. After testing for convergence, use 50 Ry for the kinetic energy cutoff of the plane-wave basis. The *k*-space and *q*-point integrations over the Brillouin zone were performed on 3 × 3 × 3 for structural relaxations and 6 × 6 × 6 for electronic structure calculations. The spin-orbit coupling (SOC) effect was also considered. The Gaussian smearing of electron density with 0.1 eV width is employed for bulk, surface, and interface, respectively.

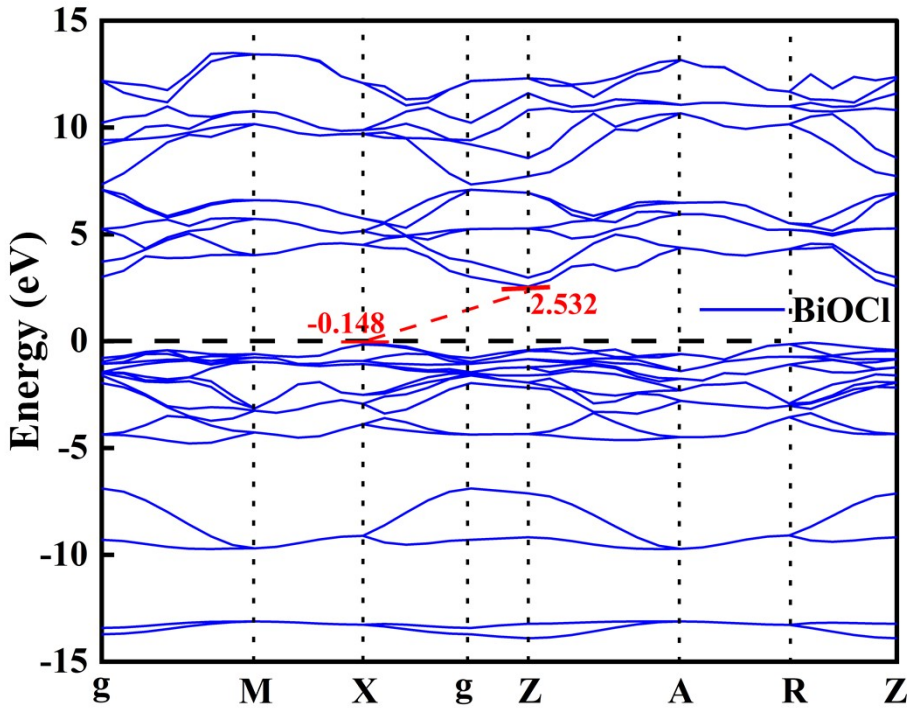


Figure S1. Band structure of BiOCl

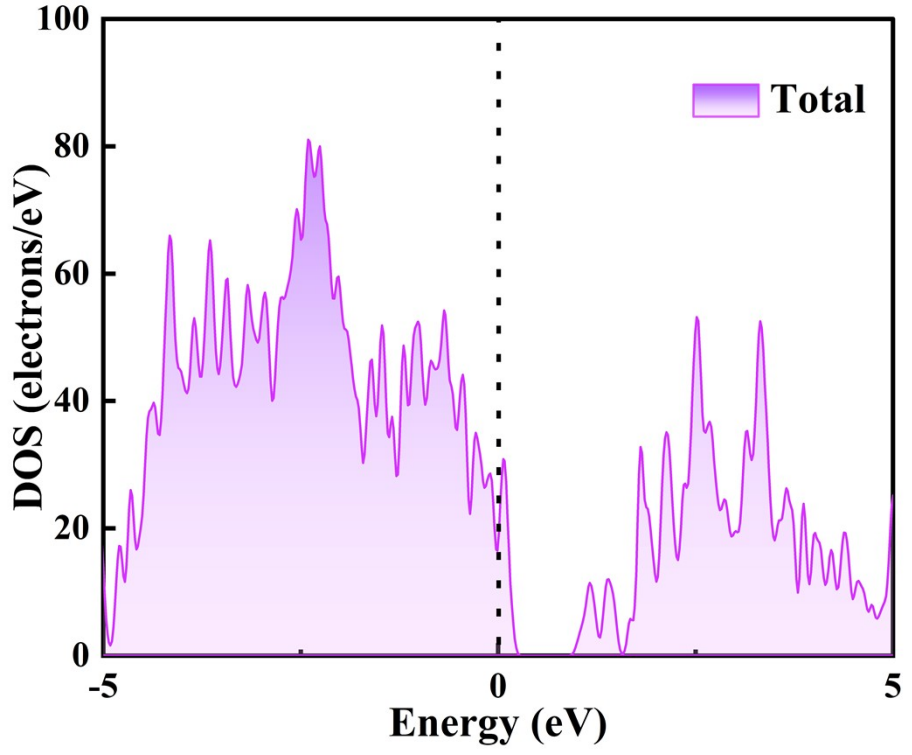


Figure S2. Total density of states (TDOS) of BiOCl/g-$C_3N_4$ heterojunction

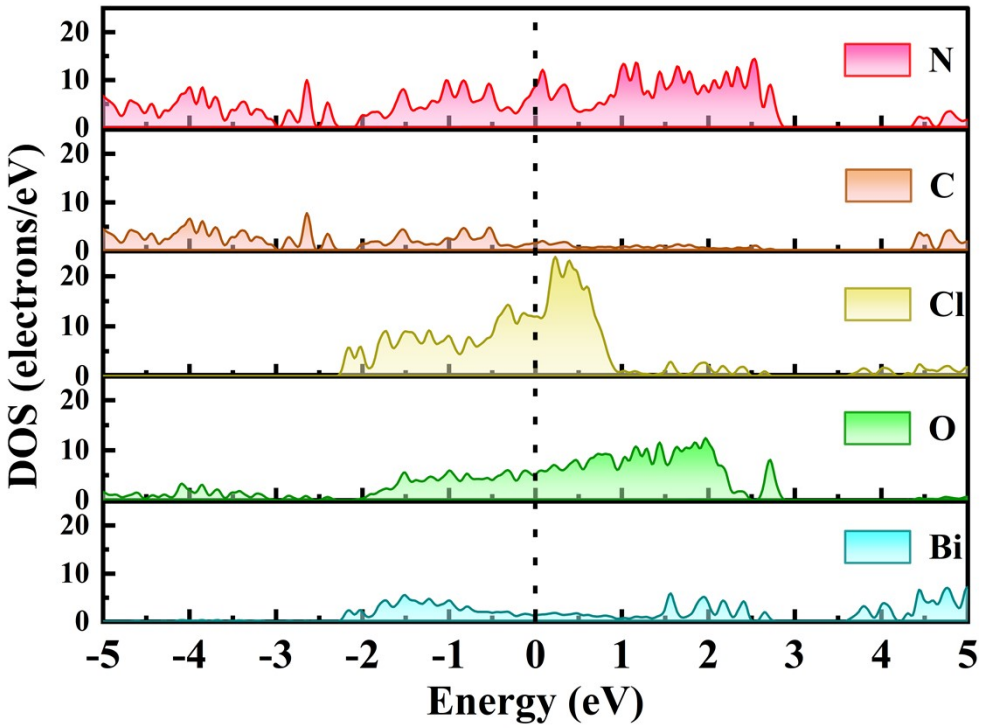


Figure S3. Partial density of states (PDOS) of each atom in BiOCl/g-$C_3N_4$ heterojunction

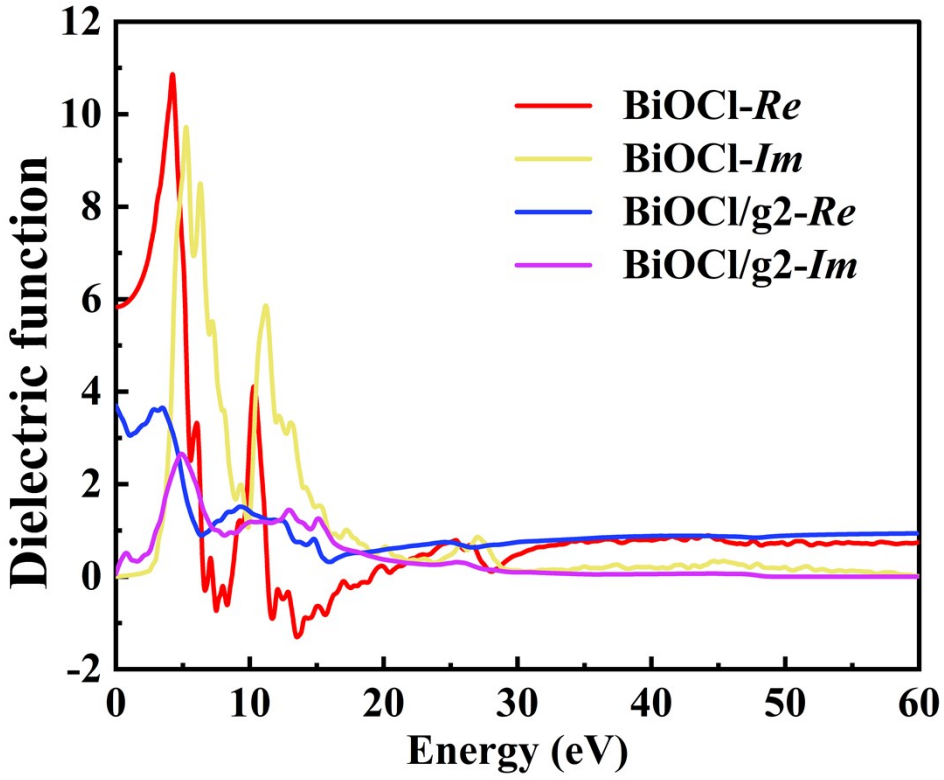


Figure S4. Real part (*Re*) and imaginary part (*Im*) of dielectric function for BiOCl and BiOCl/g-$C_3N_4$ heterojunction, respectively