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## A new understanding of the photocatalytic mechanism of the direct Z-scheme g-C3N4/TiO2 heterostructure

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### Abstract

Constructing a TiO<sub>2</sub> based heterostructure is a very effective strategy for enhancing photocatalytic performance. The details of the electronic structure, interfacial interaction, and photogenerated carrier separation are important for explaining the photocatalytic properties of a heterostructure. Herein, the density of states, charge distribution, and the band offset of the monolayer g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> heterojunction are systematically investigated through the hybrid DFT method. Results indicated that the valence band offset and the conduction band offset of the g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> heterostructure were 0.40 and 0.18 eV, respectively. Interfacial interaction made the TiO<sub>2</sub> surface with negative charge, whereas the g-C<sub>3</sub>N<sub>4</sub> surface with positive charge, which led to the formation of a built-in electric field at the interface. Under illumination, the built-in electric field accelerates the transfer of photoexcited electrons in the CB of TiO<sub>2</sub> into the VB of g-C<sub>3</sub>N<sub>4</sub>, thus resulting in the photoexcited electrons and holes naturally accumulating in the CB of g-C<sub>3</sub>N<sub>4</sub> and the VB of TiO<sub>2</sub>, respectively. The photoexcited electrons and holes gathering in different surface regions efficiently prolonged the lifetime of photogenerated carriers. Meanwhile, electrons in the CB of g-C<sub>3</sub>N<sub>4</sub> and holes in the VB of TiO<sub>2</sub> had a stronger redox ability. Therefore, g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> is a direct Z-scheme photocatalyst, and the Z-scheme heterostructure mechanism can well explain the improved photocatalytic activity of the g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> heterostructure.

### Keywords

**KeyWords Plus:** GRAPHITIC CARBON NITRIDE; TOTAL-ENERGY CALCULATIONS; WAVE BASIS-SET; VISIBLE-LIGHT; ANATASE TiO<sub>2</sub>; HYDROGEN EVOLUTION; HIGH-EFFICIENCY; H-2 EVOLUTION; PHOTOREDUCTION; PERFORMANCE

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