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

By: Liu, JJ (Liu, Jianjun)[1,2] ; Cheng, B (Cheng, Bei)[1] ; Yu, JG (Yu, Jiaguo)[1,3]

View ResearcherID and ORCID

PHYSICAL CHEMISTRY CHEMICAL PHYSICS
Volume: 18 **Issue:** 45 **Pages:** 31175-31183
DOI: 10.1039/c6cp06147h
Published: 2016
View Journal Impact

Abstract

Constructing a TiO2 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-C3N4/TiO2 heterojunction are systematically investigated through the hybrid DFT method. Results indicated that the valence band offset and the conduction band offset of the g-C3N4/TiO2 heterostructure were 0.40 and 0.18 eV, respectively. Interfacial interaction made the TiO2 surface with negative charge, whereas the g-C3N4 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 TiO2 into the VB of g-C3N4, thus resulting in the photoexcited electrons and holes naturally accumulating in the CB of g-C3N4 and the VB of TiO2, 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-C3N4 and holes in the VB of TiO2 had a stronger redox ability. Therefore, g-C3N4/TiO2 is a direct Z-scheme photocatalyst, and the Z-scheme heterostructure mechanism can well explain the improved photocatalytic activity of the g-C3N4/TiO2 heterostructure.

Keywords

KeyWords Plus: GRAPHITIC CARBON NITRIDE; TOTAL-ENERGY CALCULATIONS; WAVE BASIS-SET; VISIBLE-LIGHT; ANATASE TIO2; HYDROGEN EVOLUTION; HIGH-EFFICIENCY; H-2 EVOLUTION; PHOTOREDUCTION; PERFORMANCE

Author Information

Reprint Address: Yu, JG (reprint author)

+ Wuhan Univ Technol, State Key Lab Adv Technol Mat Synth & Proc, Wuhan 430070, Peoples R China.

Reprint Address: Yu, JG (reprint author)

+ King Abdulaziz Univ, Dept Phys, Fac Sci, Jeddah 21589, Saudi Arabia.

Addresses:

+ [1] Wuhan Univ Technol, State Key Lab Adv Technol Mat Synth & Proc, Wuhan 430070, Peoples R China

+ [2] Huaibei Normal Univ, Sch Phys & Elect Informat, Huaibei 235000, Anhui, Peoples R China

+ [3] King Abdulaziz Univ, Dept Phys, Fac Sci, Jeddah 21589, Saudi Arabia

E-mail Addresses: jiaguoyu@yahoo.com

Funding

Funding Agency	Grant Number
973 program	2013CB632402
NSFC	21433007 51372190

	21573170 51272199 51320105001
Natural Science Foundation of Hubei Province	2015CFA001
Fundamental Research Funds for the Central Universities	WUT: 2015-III-034
Innovative Research Funds of SKLWUT	2015-ZD-1

View funding text

Publisher

ROYAL SOC CHEMISTRY, THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS, ENGLAND

Categories / Classification

Research Areas: Chemistry; Physics

Web of Science Categories: Chemistry, Physical; Physics, Atomic, Molecular & Chemical

Document Information

Document Type: Article

Language: English

Accession Number: WOS:000388943500035

PubMed ID: 27819105

ISSN: 1463-9076

eISSN: 1463-9084

Journal Information

Table of Contents: Current Contents Connect

Impact Factor: Journal Citation Reports

Other Information

IDS Number: ED6CW

Cited References in Web of Science Core Collection: 62

Times Cited in Web of Science Core Collection: 9