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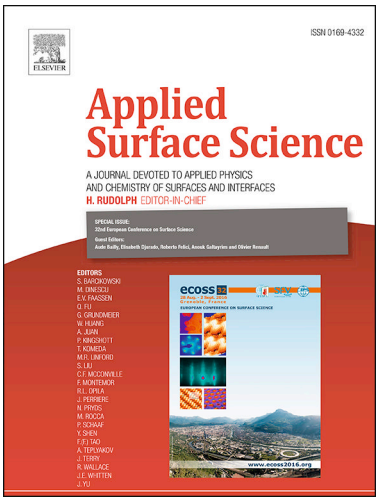

Full Length Article

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PII: S0169-4332(18)31903-2
DOI: https://doi.org/10.1016/j.apsusc.2018.07.030
Reference: APSUSC 39845

To appear in: *Applied Surface Science*

Received Date: 14 March 2018
Revised Date: 22 June 2018
Accepted Date: 4 July 2018

Please cite this article as: Y. Xing, G. Ni, J. Liu, Y. Tian, W. Que, New Insights into Photocatalytic Mechanism and Photoelectrochemical Property of Bismuth Oxybromide Heterostructure with DFT Investigation, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.07.030

New Insights into Photocatalytic Mechanism and Photoelectrochemical Property of Bismuth Oxybromide Heterostructure with DFT Investigation

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Abstract

$BiOBr/Bi_{24}O_{31}Br_{10}$ heterostructure was constructed at 500ºC by using an in-situ growth method. Results indicated that BiOBr exhibits the strongest adsorption to Rhodamine B (RhB), Tetracycline Hydrochloride (TCh) and Methyl Orange (MO), while no significant difference in adsorption to 4-Chlorophenol (4-CP) can be observed for all the samples. BiOBr shows higher photocatalytic activity for the decomposition of RhB and TCh than the $BiOBr/Bi_{24}O_{31}Br_{10}$ heterostructure, which might be attributed to its stronger adsorption and more complicated de-alkylated mechanism. However, the $BiOBr/Bi_{24}O_{31}Br_{10}$ heterostructure exhibits an enhanced visible light photocatalytic activity in degrading MO and 4-CP, which is mainly ascribed to the presence of heterojunction between BiOBr and $Bi_{24}O_{31}Br_{10}$, thus leading to an improved separation of the photoexcited electron-hole pairs, as evidenced by results of electrochemical impedance spectroscopy, photoluminescence, transient photocurrent, highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). It is also noted that the hybridized Bi 6s and Bi 6p of $Bi_{24}O_{31}Br_{10}$ make the valence band maximum be largely dispersed, and the composition of conduction band maximum contributes to the up-shift of conduction band. Based on Mott-Schottky analysis, band gap energy, VB-XPS results and density functional theory, photocatalytic mechanism of the $BiOBr/Bi_{24}O_{31}Br_{10}$ Heterostructure is also proposed.

Keywords: $BiOBr/Bi_{24}O_{31}Br_{10}$ heterostructure; in-situ growth; Photocatalytic mechanism; Density functional theory

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