Accepted Manuscript

Chalcogens doped BaTiO3 for visible light photocatalytic hydrogen production from water splitting

Hai-Cai Huang, Chuan-Lu Yang, Mei-Shan Wang, Xiao-Guang Ma

PII:	S1386-1425(18)30901-6
DOI:	doi:10.1016/j.saa.2018.09.048
Reference:	SAA 16489
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	28 February 2018
Revised date:	22 September 2018
Accepted date:	26 September 2018

Please cite this article as: Hai-Cai Huang, Chuan-Lu Yang, Mei-Shan Wang, Xiao-Guang Ma , Chalcogens doped BaTiO3 for visible light photocatalytic hydrogen production from water splitting. Saa (2018), doi:10.1016/j.saa.2018.09.048

Chalcogens doped $BaTiO_3$ for visible light photocatalytic hydrogen production from water splitting

Hai-Cai Huang, Chuan-Lu Yang*, Mei-Shan Wang, and Xiao-Guang Ma

School of Physics and Optoelectronics Engineering, Ludong University, Yantai 264025, the People's Republic of China

ABSTRACT

The pristine $BaTiO_3$ has been experimentally confirmed to catalyze hydrogen production from water splitting, but the reaction cannot be driven by the visible light because of the wide energy band gap of $BaTiO_3$. To understand the feasibility of the reaction driven by the visible light of the strongest part of the solar energy, we have investigated the effect of different concentrations of oxygen group element dopants on the electronic and optical properties of $BaTiO_3$ by using first-principles density functional theory calculations with meta-GGA+MBJ potential. The formation energy of each doped structure is calculated to examine the feasibility of synthesis in energy. The energy band gaps and the energy positions of conduction and valence bands are calculated and the results reveal that all the structures except the one that doped with 5 at % Te satisfy the conditions of water splitting although the energy band gaps of the doped $BaTiO_3$ decrease obviously. The partial charge distributions of conduct band maximum and valence band minimum are used to demonstrate the electron-hole separation. The absorption coefficients are calculated for all the considered structures. The results demonstrate that the doped chalcogens can significantly enhance the

*Corresponding author. Tel: +86 535 6672870. *E-mail address:* ycl@ldu.edu.cn. (C.L. Yang).