

## Accepted Manuscript

Title: DFT studies of elemental mercury oxidation mechanism by gaseous advanced oxidation method: co-interaction with H<sub>2</sub>O<sub>2</sub> on Fe<sub>3</sub>O<sub>4</sub> (111) surface

Authors: Changsong Zhou, Zijian Song, Zhiyue Zhang, Hongmin Yang, Ben Wang, Jie Yu, Lushi Sun



PII: S0169-4332(17)32243-2  
DOI: <http://dx.doi.org/doi:10.1016/j.apsusc.2017.07.243>  
Reference: APSUSC 36777

To appear in: *APSUSC*

Received date: 11-4-2017  
Revised date: 21-7-2017  
Accepted date: 26-7-2017

Please cite this article as: Changsong Zhou, Zijian Song, Zhiyue Zhang, Hongmin Yang, Ben Wang, Jie Yu, Lushi Sun, DFT studies of elemental mercury oxidation mechanism by gaseous advanced oxidation method: co-interaction with H<sub>2</sub>O<sub>2</sub> on Fe<sub>3</sub>O<sub>4</sub> (111) surface, *Applied Surface Science* <http://dx.doi.org/10.1016/j.apsusc.2017.07.243>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

## Essential title page information

### Title

DFT studies of elemental mercury oxidation mechanism by gaseous advanced oxidation method: co-interaction with H<sub>2</sub>O<sub>2</sub> on Fe<sub>3</sub>O<sub>4</sub> (111) surface

### Author names and affiliations

Changsong Zhou<sup>\*a</sup>, Zijian Song<sup>b</sup>, Zhiyue Zhang<sup>a</sup>, Hongmin Yang<sup>a</sup>, Ben Wang<sup>b</sup>, Jie Yu<sup>b</sup>, Lushi Sun<sup>\*b</sup>

<sup>a</sup> Engineering Laboratory of Energy System Process Conversion and Emission Reduction Technology of Jiangsu Province, School of Energy and Mechanical Engineering, Nanjing Normal University, 210042, Nanjing, China

<sup>b</sup> State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, 430074, Wuhan, China

### Corresponding author

Changsong Zhou

Address: School of Energy & Mechanical Engineering, NNU, 210042, Nanjing, China

Phone: (+86) 25-85481273; Fax: (+86) 25-85481273; E-mail: [cszhou@njjnu.edu.cn](mailto:cszhou@njjnu.edu.cn) (C. Zhou)

Lushi Sun

Address: State Key Laboratory of Coal Combustion, HUST, 430074 Wuhan, Hubei, China

Phone: (+86) 27-87542417; Fax: (+86) 27-87545526; E-mail: [sunlushi@hust.edu.cn](mailto:sunlushi@hust.edu.cn) (L. Sun)

### Present/permanent address

School of Energy and Mechanical Engineering, Nanjing Normal University, 210042, Nanjing, China

Download English Version:

<https://daneshyari.com/en/article/5349557>

Download Persian Version:

<https://daneshyari.com/article/5349557>

[Daneshyari.com](https://daneshyari.com)