

Accepted Manuscript

Full Length Article

Adsorption sensitivity of Fe decorated different graphene supports toward toxic gas molecules (CO and NO)

Zhengyang Gao, Yao Sun, Minghui Li, Weijie Yang, Xunlei Ding

PII: S0169-4332(18)31679-9
DOI: <https://doi.org/10.1016/j.apsusc.2018.06.112>
Reference: APSUSC 39620

To appear in: *Applied Surface Science*

Received Date: 11 February 2018
Revised Date: 6 June 2018
Accepted Date: 13 June 2018

Please cite this article as: Z. Gao, Y. Sun, M. Li, W. Yang, X. Ding, Adsorption sensitivity of Fe decorated different graphene supports toward toxic gas molecules (CO and NO), *Applied Surface Science* (2018), doi: <https://doi.org/10.1016/j.apsusc.2018.06.112>

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.



Adsorption sensitivity of Fe decorated different graphene supports toward toxic gas molecules (CO and NO)

Zhengyang Gao^a, Yao Sun^{a*}, Minghui Li^a, Weijie Yang^a,Xunlei Ding^{b*}

^a School of Energy and Power Engineering, North China Electric Power University, Baoding 071003, China

^b School of Mathematics and Physics, North China Electric Power University, Beijing 102206, China

Abstract

Sensitivity of Fe-decorated graphene with three different graphene-based supports (single vacancy, double vacancy and four nitrogen decorated) toward toxic gas CO and NO has been investigated by first-principles density functional theory (DFT) calculations. The adsorption configuration, adsorption energy, charge transfer, density of states, competitive behaviors of CO and NO on Fe/GN are thoroughly discussed. Furthermore, Fermi softness is investigated to evaluate the reactivity of the Fe/GN substrates surface. It is found that NO is strongly adsorbed on Fe/GN with considerable adsorption energy of 2.04~2.41eV, while CO is relatively weaker adsorbed on the same substrates with adsorption energy of 1.10~1.53eV. Based on our calculation, when CO and NO exist simultaneously, the possibility of adsorption CO can be neglected on the Fe/GN surface. In addition, Fermi softness is a good descriptor to characterize the reactivity of our Fe/GN surface. Our results could provide crucial information for adsorption sensing of NO on Fe/GN, which may be a useful clue for the design and fabrication of Fe-decorated graphene as NO sensors and adsorbent.

Key words: Fe-decorated graphene, adsorption characteristics, steric effect, Fermi softness

1. Introduction

The demand for high sensitivity, high response, high selectivity, high reliability, fast recovery, and low cost miniaturized sensors has prompted scientists to seek new gas sensing systems based on new nanomaterials. Graphene as a two-dimensional carbon sheet is an advanced material, its unique long-range π -conjugated structure brings graphene outstanding mechanical and electrical properties[1-4].

Download English Version:

<https://daneshyari.com/en/article/7833100>

Download Persian Version:

<https://daneshyari.com/article/7833100>

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