

Accepted Manuscript

First-principles approach to design and evaluation of graphene as methane sensors

Daoguo Yang, Ning Yang, Jiaming Ni, Jing Xiao, Junke Jiang, Qihua Liang, Tianling Ren, Xianping Chen



PII: S0264-1275(17)30113-2
DOI: doi: [10.1016/j.matdes.2017.01.087](https://doi.org/10.1016/j.matdes.2017.01.087)
Reference: JMADE 2728

To appear in: *Materials & Design*

Received date: 21 October 2016
Revised date: 25 January 2017
Accepted date: 27 January 2017

Please cite this article as: Daoguo Yang, Ning Yang, Jiaming Ni, Jing Xiao, Junke Jiang, Qihua Liang, Tianling Ren, Xianping Chen , First-principles approach to design and evaluation of graphene as methane sensors. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. *Jmade*(2017), doi: [10.1016/j.matdes.2017.01.087](https://doi.org/10.1016/j.matdes.2017.01.087)

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.

First-principles approach to design and evaluation of graphene as methane sensors

Daoguo Yang^{a,1}, Ning Yang^{a,*}, Jiaming Ni^a, Jing Xiao^a, Junke Jiang^a, Qihua Liang^a, Tianling Ren^c, Xianping Chen^{a,b,*}

^aThe Faculty of Mechanical and Electrical Engineering, Guilin University of Electronic Technology, 541004 Guilin, China

^bThe Key Laboratory of Optoelectronic Technology & Systems, Education Ministry of China, Chongqing University 400044, Chongqing, China.

^cInstitute of Microelectronics, Tsinghua University, 100084 Beijing, China

*Corresponding authors. E-mail addresses: xianpingchen@cqu.edu.cn (X. Chen), daoguo_yang@vip.163.com (D. Yang).

Abstract: In this work, graphene for use as methane (CH₄) sensors has been designed and evaluated via first-principles theory. Firstly, the effect of the number of layers of graphene on methane adsorption is investigated. The results show that the methane adsorption will be increased with the number of layers, the maximum energy is 0.267 eV. Furthermore, the adsorption of CH₄ leads to a small opening of the band structure of graphene. As for the doping (Al-doped) in graphene, we mainly focus on the concentration of Al atoms. The Al atom was found to cause a huge increment in methane adsorption energy that can be up to 3.212 eV when the concentration of Al atoms is 5.555%. Meanwhile, the doping of Al atoms also enhances the conductive properties of graphene. Lastly, the effect of defects was also investigated. While slightly smaller than that of pristine graphene, the methane adsorption energy of defected graphene is also increased with the number of layers. It was found that the model with the methane on the top of the empty atom and the H atoms on the top of the center of the carbon ring results in the best methane adsorption.

Keywords: adsorption; band structure; density-functional theory; methane sensor

1. Introduction

Methane (CH₄) is not only the major component of natural gas but also the main greenhouse gas, which accounts for about 20% of the global warming [1]. Methane universally exists in our daily life, such as homes, aqueous environments (wetland and ocean), mines and industries [2]. The toxic nature makes it a very dangerous gas for mankind. Therefore, the sensor for the effective detection of methane is in great need. A lot of efforts have greatly contributed to fabricate high-performance methane sensors by using metal oxides [3, 4], carbon nanotubes (CNTs) [5-7], polymers [8, 9], etc. The combined requirement for digital and non-digital functionalities in an integrated system has resulted in a dual trend in the International Technology Roadmap for Semiconductors (ITRS): miniaturization of the digital functions (“More Moore”) and functional diversification (“More-than-

Download English Version:

<https://daneshyari.com/en/article/5023718>

Download Persian Version:

<https://daneshyari.com/article/5023718>

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