UNIVERSITI TEKNOLOGI MARA

FIRST PRINCIPLES STUDY ON PROPERTIES OF DOPANTS AND DEFECTS OF PALLADIUM AND NIOBIUM WITH GAS MOLECULES ON GRAPHENE-BASED MATERIALS USING DENSITY FUNCTIONAL THEORY

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ABSTRACT

Gas monitoring technologies are in demand in the nanotech field as they are necessary for detecting flammable and hazardous gases. Graphene is widely used in sensing technology due to its fascinating electronic properties. However, the compatibility of graphene with nanoelectronic devices is low and needs to perform better due to its 2D structure and zero band gap properties. Hence, we present this theoretical study on enhancing the properties of graphene as a gas monitoring sensor in sensing lethal gas molecules to prevent air pollution. The structural and electronic properties of graphene and defect graphene upon gas molecular adsorption are determined by performing the first-principle ab initio density functional theory (DFT) calculation. The geometrical structures of graphene are optimized using DMol^3 with GGA-PBE as a functional exchange-correlation variety of gases such as carbon monoxide (CO), nitric oxide (NO), carbon dioxide (CO_2), nitrogen dioxide (NO_2) and ammonia (NH_3) are included in this study to widen the detection of toxicity gases. The gases were optimized on a graphene to find the total lowest energy. The lowest total energy indicated the minimum binding energy needed for the gas and graphene layer. The doping in the graphene layer for pristine and vacancy graphene has increased the band gap of the layer. NO_2 on Nb-doped graphene has the greatest adsorption energy, Eads= -10.212 eV, with 2.118 Å distance of NO_2 molecule to the graphene surface. Using the Mulliken calculation, the charge transfer for NO_2 on NbG also has the highest value, ΔQ= -0.483 e. For gas molecules on vacancy graphene, the NO molecule on vacancy graphene has the greatest adsorption energy value, Eads= -6.756 eV, with the distance between the molecule to the graphene surface, d= 3.658 Å. The charge transfer on NO_2 on Nb-doped vacancy graphene is the highest, with -0.448 e. From these findings, the doping of Nb and the vacancy defect increase the band gap of the graphene surface. The study aims to find the potential of doped and defective graphene for molecule sensor applications.

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CHAPTER ONE
INTRODUCTION

1.1 Background Study

In current scenario, monitoring of produced gases are very important in industrial field around the world. From home appliances such as air conditioners to electric chimneys and safety systems at industries of gases monitoring, the sensor is needed [1]–[10]. It is a necessary device in industrial because of its capability in detecting fatal, harmful, and flammable gases. Gas sensor is demanded because of its electrochemical technology, less-expensive option that offers high accuracy, low power requirements, and sensitivity to a particular gas in parts-per-million (ppm) range [11]–[13].

Moreover, gas sensors are available in wide specifications depending on the sensitivity level, type of gas to be sensed, physical dimensions and numerous other factors. Most of the commercial gas detector are based on metal oxide semiconductor, polymer materials [14]–[16]. The systems used for sensing are optical methods, calorimetric method, gas chromatography and acoustic method by Gupta *et al* [17]. Furthermore, Varghese *et al* [18] has stated that there are a few limitations of the gas sensor such as:

i) costly
ii) sensitivity in part per billion (ppb) is uncommon
iii) poor selectivity
iv) limited of lifetime
v) poor repeatability
vi) miniaturization is challenging
vii) high power consumption

Nowadays, air pollution is one of the global challenges that critically arise and need to be controlled. The technology that can detect the poisonous and toxicity of gases