CHAPTER I

Introduction

In today's world, there exist various kinds of threats in the form of dangerous gases or chemicals. These threats are serious problem, which can cause many long-term chronic health effects, particularly to people living around industrial areas [1,2]. Thus, the possibility for detection of gas leaks in a hazardous work environment has now become a fundamental issue involving safety, environmental and health risk. To keep the society safe, we need an effective gas sensor which is able to detect one atom/molecule of the gas. We believe nowadays that the potentials of nanotechnology become a promising way to overcome the limiting factor of gas sensors in improving selectivity and sensitivity and response time.

Two-dimensional nanostructure materials have taken the front row in innovative applications in the last decade after the successful experimental exfoliation of graphene. Gas sensors based on graphene have attracted much attention since graphene has excellent sensitivity to detect various gas molecules, large sensing area per unit volume, low electronic temperature noise, fast response time and high chemical stability [3,4]. The potential use of graphene for gas detection has been intensively investigated both experimentally [5-6] and theoretically [8-10]. However, growth of graphene over large surface areas is constrained. This motivated the search for other materials with similar favorable properties. In turn, this has led to the discovery of silicene as a silicon counterpart. The good properties with versatile silicon based nanotechnology gives the edge to silicene rather than graphene. This serves as the motivation of our work to theoretically explore the applicability of silicene for gas sensing.

The massless Dirac Fermions are the main reasons behind the ultrahigh carrier mobility for both the honeycomb structures of silicene and graphene [11-12]. Geometrically, the hexagonal structure of silicene has a larger size due to the larger ionic radius of Si atoms [13], but they have similar electronic structures. One important demarcation between the two structures is a buckled formation in silicene. This is due to sp^3 and sp^2 hybridization [14] rather than only sp^2 hybridization. This feature leads to a few prominent differences in the properties of silicene and graphene. Band gap tuning with an external electric field [15-17] and with the binding adsorbates [18-20] can be seen more profoundly in silicene than in graphene [21]. Although free-standing silicene has not been achieved so far, recent progress shows that it can be synthesized experimentally by depositing silicon on different surfaces such as silver [22] gold [23], zirconium diboride [24] and iridium [25].

To date, a wide range of potential applications of silicene have been proposed in various field such as spintronics [26-28], FETs [29-31], hydrogen storage [32,33] and sensing devices [34,35]. Nevertheless, using silicene as gas sensor has not been given the attention it deserves. Two theoretical investigations based on the density functional theory (DFT) were done to explore potential application of silicene as a molecular sensor for gas molecules [36,37]. They revealed changes in the electronic structures of silicene with adsorbed gas. The prime parameters to characterize the sensor performance of a gas sensor are sensitivity, selectivity, response time and recovery time. They should be addressed simultaneously to meet real application requirements of silicene based sensing systems.

The purpose of our study was therefore twofold. Firstly, we used the state-of-the-art first-principle methods to study the electronic and transport properties to evaluate the gas discrimination of silicene in terms of sensitivity and selectivity. Secondly, we demonstrate the possibility to improve gas sensing performance of silicene through doping this material with B and N atoms.

In this work, we investigated the electronic and transport properties of gas molecules adsorbed onto pristine (P) and B/N-doped silicene by employing a robust combination of non-equilibrium Green's function (NEGF) techniques and DFT. Four representative gas species; i.e., NO_2, NO, NH_3 and CO molecules, which are of main interest for environmental safety and medical purposes, were shown to be detectable by silicene based sensor devices. The sensitivity and selectivity of the devices to the presence of those gas molecules were evaluated from the changes in their electronic transport properties. Our results indicate that doping impurity atoms into silicene can enhance the interaction between the gas molecules and doped devices. This enabled an immense improvement in the performance of this type of sensor.