Journal of Basrah Researches (Sciences) **51**(2), 284 (2025)
DOI: https://doi.org/10.56714/bjrs.51.2.20

Model Calculation for the Chemisorption of Li and Na Atoms on Bilayer Graphene

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ARTICLE INFO

Received 21 October 2025
Revised 13 December 2025
Accepted 22 December 2025
Published 31 December 2025

Keywords:

Bilayer Graphene, Chemisorption, Anderson-Newns Model.

Citation: B. M. Ajer , A. R. Ahmed. , J. Basrah Res. (Sci.) **50**(2), 284 (2025). DOI:https://doi.org/10.56714/bjrs.51.2.20

ABSTRACT

The Anderson-Newns model is used to study the chemisorption process of lithium and sodium atoms on bilayer graphene. The density of states of bilayer graphene is employed, along with the effects of quantum coupling represented by broadening and quantum shift to calculate the electronic properties, magnetization and chemisorption energy. The self-consistent solutions of the atomic occupation numbers revealed that the solution is magnetic at relatively large distances from bilayer graphene, and turn into non-magnetic one at certain close distance. The relationship between the magnetization of atoms and their distance from bilayer plane can be exploited in spintronics applications. Moreover, the ionic contribution to the chemisorption energy dominates at closest approach distances, providing a clear description of the bonding nature with bilayer graphene. These results can take advantage for experimental applications in storage of null magnetization atoms on two dimensional materials.

1. Introduction

Bilayer graphene consists of two layers of graphene stacked together. Each graphene layer is a single sheet of carbon atoms arranged in a hexagonal lattice. When these two layers are placed on top of each other, they form bilayer graphene, which has some unique properties as compared to monolayer graphene [1,2]. Many of the properties of bilayer graphene are similar to those in monolayer [3], such as high electrical conductivity with room temperature mobility up to 40.000 cm2 V-1 S-1 in air [4]; electrical properties can be tuned by doping or changing the carrier density through gating [5]; additionally, high thermal conductivity at room temperature (about 2,800Wm−1K−1)[6]; strength flexibility and mechanical stiffness (Young's modulus is about 0.8 TPa) [7]; transmittance of white light of about 95% with transparency ; impermeability to gases [8]. Therefore, bilayer graphene will possess potential for multiple applications in various fields, such as flexible and transparent electrodes for touch screens, thermoelectric devices, high-frequency transistors, photodetectors, photonic devices, and batteries [9].

The bilayer graphene gap can be tuned through chemical modification from zero up to values typical for conventional semiconductors like silicon or GaAs[10]. In transistors made of graphene, the junction does not close, and this problem is solved by using bilayer graphene because there is a real gap in it [10-13]. Bilayer graphene can be formed by stacking two graphene sheets, rotating one relative to the other. Depending on the twisting angle, this material exhibits magnetic properties, superconductivity, and various other electronic phenomena [14-17]. Some researchers have

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ISSN: 1817-2695 (Print); 2411-524X (Online)
Online at: https://jou.jobrs.edu.iq