Applied Surface Science 256 (2010) 5783–5788

Contents lists available at ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Structural and electronic properties of H-passivated graphene

A.Z. AlZahrani[a,*], G.P. Srivastava[b]

[a] *Physics Department, Faculty of Science, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia*
[b] *School of Physics, University of Exeter, Stocker Road, Exeter EX4 4QL, UK*

ARTICLE INFO

Article history:
Available online 29 March 2010

Keywords:
Graphene
Graphane
Density functional theory
Local density approximation
Pseudopotential method
Hydrogen passivation

ABSTRACT

The atomic and electronic structures of graphane (*hydrogen-passivated graphene*) are theoretically investigated using the local density approximation (LDA) of the density functional theory (DFT) and the pseudopotential method. Our total energy calculations suggest that the chairlike configuration for graphane is more energetically stable than the boatlike and tablelike configurations by approximately 0.129 eV/cell and 0.655 eV/cell, respectively. Our calculations suggest that the LDA band gap of the chairlike structure is approximately 3.9 eV. The equilibrium geometry and the band structure of the chairlike conformer are investigated and compared with the available experimental and theoretical data. We further present total and partial charge density to reveal the orbital nature of the highest occupied and the lowest unoccupied states.