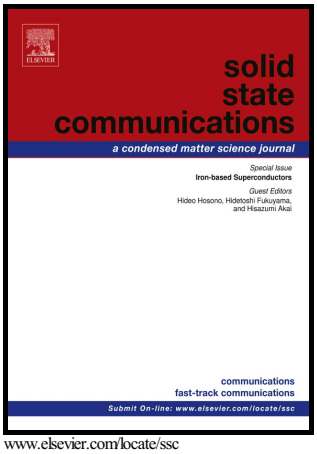

www.elsevier.com/locate/ssc

Mechanical and electric properties of graphitic carbon nitride sheet: First-principles calculations

Yusuf Zuntu Abdullahi, Tiem Leong Yoon, Mohd Mahadi Halim, Md. Roslan Hashim, Thong Leng Lim

PII: S0038-1098(16)30266-6
DOI: http://dx.doi.org/10.1016/j.ssc.2016.10.005
Reference: SSC13054

To appear in: *Solid State Communications*

Received date: 29 June 2016
Revised date: 13 September 2016
Accepted date: 4 October 2016

Cite this article as: Yusuf Zuntu Abdullahi, Tiem Leong Yoon, Mohd Mahadi Halim, Md. Roslan Hashim and Thong Leng Lim, Mechanical and electri properties of graphitic carbon nitride sheet: First-principles calculations, *Soli State Communications,* http://dx.doi.org/10.1016/j.ssc.2016.10.005

Mechanical and electric properties of graphitic carbon nitride sheet: First-principles calculations

Yusuf Zuntu Abdullahi[a,c*], Tiem Leong Yoon[a], Mohd Mahadi Halim[a], Md. Roslan Hashim[b], Thong Leng Lim[d]

[a]School of Physics, Universiti Sains Malaysia, 11800 Penang, Malaysia
[b]Institute of Nano-Optoelectronics Research and Technology Laboratory, Universiti Sains Malaysia, 11900 Penang, Malaysia
[c]Department of Physics, Faculty of Science, Kaduna State University, P.M.B. 2339 Kaduna State, Nigeria
[d]Faculty of Engineering and Technology, Multimedia University, Jalan Ayer Keroh Lama, 75450 Melaka, Malaysia
[*]Corresponding author. Email address: *yzunt@yahoo.com*

Abstract

In this work, mechanical properties, elastic constants and the strain responses on the electronic properties of graphitic heptazine are investigated using density functional theory. The computed lattice constant and bulk modulus are in good agreement with the available literatures. The in-plane stiffness compared well with a similar two-dimensional structure, whereas the Poisson's ratio is half that of graphene. The calculated critical points (elastic and yielding points) for both the uni- and bi-axial strains show that the heptazine material can withstand longer tensions in the plastic region. This shows that the heptazine sheet is mechanically stable. Our calculations also predict enhanced band gap induced by small amount of bi-axial tensile strain within the elastic region. The increase in band gap is a result of symmetric deformations which predominantly affect the structural features of the sheet, leading to the eventual reorientation in the atomic orbitals of the sheet. We find no change in the electric properties of the sheet under electric field up to a peak value of 10 V/nm. Such properties may serve as a guide for future nanodevice applications.

Keywords: Heptazine; Density Functional Theory; Mechanical properties; Electric properties.

1. Introduction

Graphitic two dimensional (2D) monolayers of carbon materials continue to demonstrate superior technological advantage due to their numerous excellent physical properties [1].