

Accepted Manuscript

Energetic and electronic structure of penta-graphene nanoribbons

Biplab Rajbanshi, Sunandan Sarkar, Bikash Mandal, Pranab Sarkar

PII: S0008-6223(16)30014-8

DOI: [10.1016/j.carbon.2016.01.014](https://doi.org/10.1016/j.carbon.2016.01.014)

Reference: CARBON 10645

To appear in: *Carbon*

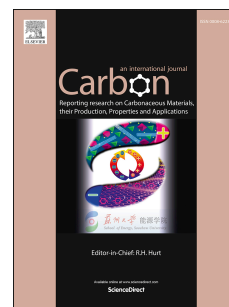
Received Date: 12 September 2015

Revised Date: 31 December 2015

Accepted Date: 6 January 2016

Please cite this article as: B. Rajbanshi, S. Sarkar, B. Mandal, P. Sarkar, Energetic and electronic structure of penta-graphene nanoribbons, *Carbon* (2016), doi: 10.1016/j.carbon.2016.01.014.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Energetic and electronic structure of penta-graphene nanoribbons

Biplab Rajbanshi, Sunandan Sarkar, Bikash Mandal, Pranab Sarkar*

Department of Chemistry, Visva-Bharati University, Santiniketan- 731235, India

Abstract

Inspired by a very recent theoretical work on penta-graphene, a two dimensional (2D) carbon sheet [Proc. Nat. Acad. Sci. **2015**, *112*, 2372] composed of only carbon pentagons, we have made an attempt to see the stability and electronic properties of its one dimensional (1D) ribbons, naming penta-graphene nanoribbon (pentaGNR). Our first principle calculations predict that, pentaGNR is dynamically stable; it is mechanically flexible tolerating upto 11.5% of axial strain. We have also explored the electronic properties of the nanoribbons with different widths which show interesting charge separation for wider ribbons. The band gap of wider ribbons changes only marginally with further increasing the ribbon width which opens up the possibility of a stable nanoribbon with large band gap which is very useful for designing optoelectronic devices.

*Corresponding author

Email address: pranab.sarkar@visva-bharati.ac.in (Pranab Sarkar)

Download English Version:

<https://daneshyari.com/en/article/7850114>

Download Persian Version:

<https://daneshyari.com/article/7850114>

[Daneshyari.com](https://daneshyari.com)