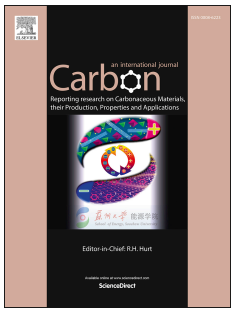
Accepted Manuscript



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PII: S0008-6223(16)30329-3

DOI: 10.1016/j.carbon.2016.04.058

Reference: CARBON 10939

To appear in: *Carbon*

Received Date: 21 December 2015

Revised Date: 27 March 2016

Accepted Date: 25 April 2016

Please cite this article as: X. Zhang, L. Wei, J. Tan, M. Zhao, Prediction of an ultrasoft graphene allotrope with Dirac cones, *Carbon* (2016), doi: 10.1016/j.carbon.2016.04.058.

Prediction of an ultrasoft graphene allotrope with Dirac cones

Xiaoming Zhang[1], Lin Wei[1,2], Jie Tan[1], Mingwen Zhao*[1]

[1]*School of Physics and State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, Shandong, China.*

[2]*School of Information Science and Engineering, Shandong University, Jinan 250100, Shandong, China.*

Abstract

Searching for the Dirac materials with ultrasoftness is crucial for flexible electronics applications. Based on first-principles calculations, we propose a new carbon allotrope (named as ph-graphene) with a penta-hexagonal framework, which is energetically more favorable than the penta-graphene composing surely of pentagons and some of already-synthesized carbon allotropes. Ph-graphene has an in-plane stiffness of 27.75 *GPa·nm*, smaller than those of graphene and penta-graphene by one order. The famous isotropic Dirac cones are well preserved in the ultrasoft ph-graphene, exhibiting delocalized feature of p_z orbits with the Fermi velocity of 2.8×10^5 *m/s*. Additionally, surface hydrogenation alters drastically the electronic and mechanical properties of ph-graphene, resulting in electronic spin-polarization and anisotropic negative Poisson's ratios sequentially with the increase of hydrogenation concentrations.

*Corresponding author. Tel: 86-531-88364655. E-mail: zmw@sdu.edu.cn (Mingwen Zhao)