

Accepted Manuscript

Hydrogenated black phosphorus single layer

Mohammed Moaied, Jisang Hong

PII: S1386-9477(18)30298-4

DOI: [10.1016/j.physe.2018.07.013](https://doi.org/10.1016/j.physe.2018.07.013)

Reference: PHYSE 13216

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

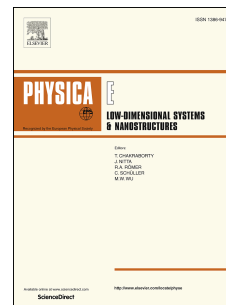
Received Date: 26 February 2018

Revised Date: 22 April 2018

Accepted Date: 12 July 2018

Please cite this article as: M. Moaied, J. Hong, Hydrogenated black phosphorus single layer, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: 10.1016/j.physe.2018.07.013.

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.



Hydrogenated Black Phosphorus Single Layer

Mohammed Moaied

Department of Physics, Pukyong National University, Busan 608-737, Korea

Department of Physics, Faculty of Science, Zagazig University, 44519 Zagazig, Egypt

Jisang Hong,*

Department of Physics, Pukyong National University, Busan 608-737, Korea

ABSTRACT

Using the first principles calculations, we investigated the physical properties of hydrogenated black phosphorene layer. For a single H adsorption, the P top site became the most stable adsorption position and this impurity adsorption created a broken P-P bond. Due to this broken bond, the adsorption of a single hydrogen atom on a phosphorene layer induced a total magnetic moment at about $1.0 \mu_B$ and that the spin-polarized state was mainly localized around the dangling phosphorus atom. In the hydrogenated system, the hydrogen atoms preferred the different sublattice adsorption at rather short H-H inter-atomic distance ($\sim 3.5 \text{ \AA}$) while the sublattice dependent formation energy was greatly suppressed at larger than H-H distance of 3.5 \AA . We obtained that the hydrogenated phosphorene layer displayed an antiferromagnetic state until the H-H inter-atomic distance became around 8 \AA and the energy difference between ferromagnetic (FM) and antiferromagnetic (AFM) states almost vanished beyond this interatomic distance. This result may suggest that the hydrogenated phosphorene layer system shows an antiferromagnetic state at high H concentration while the exchange coupling is greatly suppressed at low H concentration. Thus, it will be possible to manipulate the magnetic property by applying even small magnetic field at low H concentration and this can feature can be utilized for spintronics applications.

Keywords: ab initio, Adsorption, Hydrogen, Black phosphorus, Magnetic properties.

Download English Version:

<https://daneshyari.com/en/article/11006908>

Download Persian Version:

<https://daneshyari.com/article/11006908>

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