


# Document details

1 of 1

[Export](#) [Download](#) [Print](#) [E-mail](#) [Save to PDF](#) [Add to List](#) [More...](#) ▸[Full Text](#) [View at Publisher](#)

Journal of Computational and Theoretical Nanoscience  
Volume 11, Issue 1, January 2014, Pages 58-61

## Density functional study of spin polarization on a carbon material with a hexagonal structure induced by iron atoms (Article)

Muhida, R.<sup>a</sup>, Rahman, M.M.<sup>b</sup>, Chowdhury, M.S.H.<sup>c</sup>, Setiyanto, H.<sup>d</sup>, Zainuddin, H.<sup>de</sup>, Azmi, B.Z.<sup>dt</sup>, Kasai, H.<sup>ef</sup> 

<sup>a</sup>Department of Physics, Surya College of Education (STKIP Surya), Gedung SURE, Jl. Scientia Boulevard Blok U/7, Gading Serpong, Tangerang 15810, Banten, Indonesia

<sup>b</sup>Department of Physics, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

<sup>c</sup>Department of Science in Engineering, Faculty of Engineering, International Islamic University Malaysia, P.O. Box 10, 50728 Kuala Lumpur, Malaysia

[View additional affiliations](#) ▾

### Abstract

[View references \(25\)](#)

We investigate the spin polarization of a non magnetic material, e.g., a carbon material made from ten C atoms forming a hexagonal structure with total spin  $S = 0$ , induced by a ferromagnetic material, e.g., two Fe atoms with a total spin  $S = 4$ . Based on the density functional theory, we calculate the total spin density of the system. Our preliminary results show that the total spin for the ten C atoms changes from  $S = 0$  to  $S = 4$ , while the total spin of the two Fe atoms changes from  $S = 4$  to  $S = 0$ . These results seem to indicate that there is a promising possibility to induce spin polarization on a carbon material by Fe atoms.

Copyright © 2014 American Scientific Publishers All rights reserved.

### Author keywords

[Carbon Material](#) [Density Functional Theory](#) [Ferromagnetic Material](#) [Scanning Tunneling Microscopy](#) [Spin Polarization](#)

### Indexed keywords

[A-carbon](#)  
[Carbon material](#)  
[Density-functional study](#)  
[Fe atoms](#)  
[Hexagonal structures](#)  
[Iron atoms](#)  
[Non-magnetic materials](#)  
[Spin densities](#)

Engineering controlled terms:

[Atoms](#) [Carbon](#) [Ferromagnetic materials](#) [Scanning tunneling microscopy](#) [Spin polarization](#)

Engineering main heading:

[Density functional theory](#)

### Funding details

Funding number	Funding sponsor	Acronym
	Ministry of Education, Culture, Sports, Science, and Technology	MEXT
	Japan Society for the Promotion of Science	JSPS


ISSN: 15461955  
Source Type: Journal  
Original language: English

DOI: 10.1166/jctn.2014.3317  
Document Type: Article

[Metrics](#) ⓘ [View all metrics](#) ▸

1  **Citation in Scopus**  
20th Percentile

0.15  **Field-Weighted Citation Impact**

 **PlumX Metrics** ▾  
Usage, Captures, Mentions, Social Media and Citations beyond Scopus.

### Cited by 1 document

Density functional study of structural stabilities, electric and magnetic properties of vanadium adsorption on graphene

Rahman, M.M., Abdullahi, Y.Z., Shuaibu, A.  
(2015) *Journal of Computational and Theoretical Nanoscience*

Inform me when this document is cited in Scopus:

[Set citation alert](#) ▸[Set citation feed](#) ▸

### Related documents

Stable structures of Fe nanowires on Cu(111)

Kishi, T., Nakanishi, H., Kasai, H.  
(2003) *Japanese Journal of Applied Physics, Part 1: Regular Papers and Short Notes and Review Papers*

Magnetic properties of Fe nanowires on Cu(111)

Kishi, T., Nakanishi, H., Kasai, H.  
(2003) *Shinku/Journal of the Vacuum Society of Japan*

Transport and magnetic properties of magnetic alloy atom bridge

Nakanishi, H., Kasai, H., Kishi, T.  
(2003) *Physica E: Low-Dimensional Systems and Nanostructures*

[View all related documents based on references](#)

Find more related documents in Scopus based on:

[Authors](#) ▸ [Keywords](#) ▸