Theoretical investigation of manganese adsorption on graphene and graphane: A first-principles comparative study

By: AlZahrani, AZ (AlZahrani, A. Z.)

View ResearcherID and ORCID

PHYSICA B-CONDENSED MATTER
Volume: 407 **Issue:** 6 **Pages:** 992-1002
DOI: 10.1016/j.physb.2011.12.127
Published: MAR 15 2012
View Journal Impact

Abstract

Within the framework of spin-polarized generalized gradient approximation (sigma GGA) of the density functional theory (DFT) and pseudopotential method, the structural, magnetic, and electronic properties of graphene and graphane upon the adsorption of manganese atoms have been theoretically investigated. In contrast to the recent results (New J. Phys. 12, 063020 (2010)), Mn atom has been found to be adsorbed on a hollow-site configuration and no appreciable indication to substitute one of the C atoms of the graphene sheet. Unlike the recent results on Mn-doped graphane (Carbon 48, 3901 (2010)), the Mn adatom prefers to adsorb on the top of a carbon atom, forming a bridge with the uppermost hydrogen atoms. The magnetic moment of the Mn-doped graphene is found to be larger than that of the Mn-doped graphane. The structural parameters and electronic properties of both Mn-doped graphene and Mn-doped graphane are determined and compared with the available data. (c) 2011 Elsevier B.V. All rights reserved.

Keywords

KeyWords Plus: ELECTRONIC-PROPERTIES; GRAPHITE; SEMICONDUCTORS; NANOTUBES; CARBON

Author Information

Reprint Address: AlZahrani, AZ (reprint author)

+ King Abdulaziz Univ, Fac Sci, Dept Phys, POB 80203, Jeddah 21589, Saudi Arabia.

Addresses:

+ [1] King Abdulaziz Univ, Fac Sci, Dept Phys, Jeddah 21589, Saudi Arabia

E-mail Addresses: azalzahrani@kau.edu.sa

Funding

Funding Agency	Grant Number
King Abdulaziz University (KAU)	23/130/1431

View funding text

Publisher

ELSEVIER SCIENCE BV, PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS

Categories / Classification

Research Areas: Physics

Web of Science Categories: Physics, Condensed Matter

Document Information

Document Type: Article

Language: English

Citation Network

Accession Number: WOS:000301043000010

ISSN: 0921-4526

eISSN: 1873-2135

Journal Information

Table of Contents: Current Contents Connect
Impact Factor: Journal Citation Reports

Other Information

IDS Number: 902MQ

Cited References in Web of Science Core Collection: 56

Times Cited in Web of Science Core Collection: 15