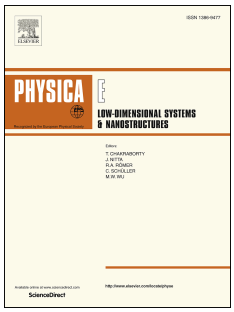
Accepted Manuscript



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PII: S1386-9477(18)30486-7

DOI: 10.1016/j.physe.2018.07.017

Reference: PHYSE 13220

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

Received Date: 30 March 2018

Revised Date: 13 July 2018

Accepted Date: 16 July 2018

Please cite this article as: O. Omeroglu, E. Kutlu, P. Narin, S.B. Lisesivdin, E. Ozbay, Electronic properties of graphene nanoribbons doped with zinc, cadmium, mercury atoms, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: 10.1016/j.physe.2018.07.017.

Electronic Properties of Graphene Nanoribbons Doped with Zinc, Cadmium, Mercury Atoms

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Abstract

The effect of substitutional impurities as Zinc (Zn), Cadmium (Cd) and Mercury (Hg) on electronic properties of graphene nanoribbons (GNRs) was investigated by using Density Functional Theory (DFT). A substantial change in the electronic properties of GNR structures was observed while changing the position of dopant atom from the edge to the center of armchair graphene nanoribbons (AGNRs) and zigzag graphene nanoribbons (ZGNRs). The calculations are shown that the electronic band gap of GNRs can be controlled depending on the position of dopant atoms. The calculated electronic band structures for both AGNRs and ZGNRs show spin-dependent metallic or semiconductor behavior according to the position of dopant atoms. From the Density of States (DOS) information, quasi-zero-dimensional (Q0D) and quasi-one-dimensional (Q1D) type behaviors are observed. It is shown that because the doped ZGNRs had the lowest total energies, ZGNRs are energetically more stable than AGNRs.

Keywords: Graphene nanoribbon, Doping, DFT, Zinc, Cadmium, Mercury

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1. Introduction

Graphene is two-dimensional material established by a sheet of carbon (C) atoms arranged in order a hexagonal lattice. It is an allotrope of carbon in the structure of a plane of sp^2 bonded atoms with a molecule bond length of 0.142 nanometers, has emerged as an interesting material of the 21st century [1]. Graphene and its different types have the potential to be used in various applications impact on electronic and optoelectronic devices, chemical sensors, nanocomposites, and energy storage [2, 3]. Graphene can be seen as the fundamental essential principle of a kind of materials with different dimensionalities, such as one-dimensional nanoribbons or nanotubes, zero-dimensional fullerenes or three-dimensional graphite [4-6]. The first of these, graphene nanoribbons are one-dimensional structures. ZGNR and AGNR are classified as zigzag and