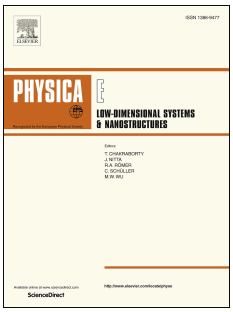
Accepted Manuscript



Density functional theory study of adsorption properties of non-carbon, carbon and functionalized graphene surfaces towards the zinc and lead atoms

A. Hamed Mashhadzadeh, M. Ghorbnzadeh Ahangari, A. Salmankhani, M. Fataliyan

PII: S1386-9477(18)30096-1

DOI: 10.1016/j.physe.2018.08.010

Reference: PHYSE 13255

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

Received Date: 18 January 2018

Revised Date: 12 June 2018

Accepted Date: 8 August 2018

Please cite this article as: A. Hamed Mashhadzadeh, M. Ghorbnzadeh Ahangari, A. Salmankhani, M. Fataliyan, Density functional theory study of adsorption properties of non-carbon, carbon and functionalized graphene surfaces towards the zinc and lead atoms, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: 10.1016/j.physe.2018.08.010.

Density functional theory study of adsorption properties of non-carbon, carbon and functionalized graphene surfaces towards the zinc and lead atoms

A. Hamed Mashhadzadeh[1*], M. Ghorbnzadeh Ahangari[2], A. Salmankhani[3], M. fataliyan[4]

[1]*Department of Mechanical Engineering, Sari Branch, Islamic Azad University, Sari, Iran*
[2]*Department of Mechanical Engineering, Faculty of Engineering and Technology, University of Mazandaran, Babolsar, Iran*
[3] *Department of Mechanical Engineering, KN University of technology, Tehran, Iran*
[4]*Department of Mechanical Engineering, Semnan Branch, Islamic Azad University, Semnan, Iran*

Abstract:

In the current study, we Investigated the adsorption properties of zinc (Zn) and lead (Pb) atoms on the surface of carbonic and non-carbonic graphene using Density functional theory calculations. The procedure for this research can be divided into two sections. First, we calculated the adsorption value of single zinc and lead atoms with such non-carbonic graphene-like structures as Boron-Nitride (BN), Aluminum-Nitride (AlN), Gallium-Nitride (GaN), Silicon-Carbide (SiC), and Silicene. We found that the silicene was more powerful to detect the stated heavy metal atoms compared with others. The calculated adsorption values between the single zinc and lead atoms with silicene monolayer sheet were equal to -0.90 eV and -3.80 eV, respectively. We also used electron transfer caculations after adsorbing the stated heavy metal atoms and found that the calculated charge transfer was equal to 0.42 and 0.12 electrons for Silicene/Pb and Silicene/Zn complex, respectively. The density of states (DOS) results demonstrated that a strong hybridization could occur between the Pb atom and the silicene graphene. Then, we performed DFT calculations to determine the interaction energy between the mentioned metal atoms with pristine carbonic grapheme. We found that the interaction in graphene/Zn (-0.09 eV) and graphene/Pb (-0.45 eV) was so weak, especially for graphene and zinc. To overcome this issue, we first activated the surface of graphene by carboxyl and hydroxide group. The interaction energy values between the zinc and lead atoms with graphene-COOH were approximately -0.18 eV and -1.01 eV, respectively, which showed improvements in the adsorption energy. Then, we approached the mentioned metal atoms on the surface of –OH-decorated graphene and demonstrated that the interaction energy between the single zinc and lead atoms with graphene-OH were about -0.78 eV and -3.33 eV. In other words, it improved by 755% and 623% compared with graphene/Zn and graphene/Pb, respectively. The strong adsorption between the hydroxyl group and the stated metals atom caused the OH group to be isolated from the graphene surface and become an individual molecule.

Keywords: Graphene; DFT; Adsorption; Functionalization; Heavy metal atoms

*Corresponding author: Tel./fax: +98 1135305108**.**

E-mail address: amin.hamed.m@gmail.com; amin.hamedmashhadzadeh@yahoo.com