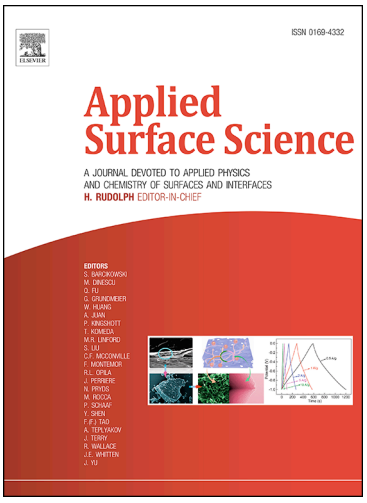

Full Length Article

Electronic and magnetic properties of the adsorption of As harmful species on zero-valent Fe surfaces, clusters and nanoparticules

Leslie L. Alfonso Tobón, Silvia Fuente, María M. Branda

PII: S0169-4332(18)32625-4
DOI: https://doi.org/10.1016/j.apsusc.2018.09.199
Reference: APSUSC 40503

To appear in: *Applied Surface Science*

Received Date: 5 July 2018
Revised Date: 13 September 2018
Accepted Date: 24 September 2018

Please cite this article as: L.L. Alfonso Tobón, S. Fuente, M.M. Branda, Electronic and magnetic properties of the adsorption of As harmful species on zero-valent Fe surfaces, clusters and nanoparticules, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.09.199

Electronic and magnetic properties of the adsorption of As harmful species on zero-valent Fe surfaces, clusters and nanoparticules.

Leslie L. Alfonso Tobón[1], Silvia Fuente[1] and María M. Branda[2,*]

[1] IFISUR, CONICET. Av. Alem 1253-Bahía Blanca (8000). Argentina

[2] INFAP, CONICET. Av. Ejército de los Andes 950- Ciudad de San Luis (5700). Argentina

*Corresponding author. E-mail address: mariamartabranda@gmail.com

Keywords: water contaminants, As species, adsorption, iron, electronic properties.

Abstract

A systematic theoretical study of the adsorption of H_3AsO_3 and H_3AsO_4 acids on Fe nanoparticles was carried out using the Density Functional Theory (DFT). Different sizes of zero-valent iron particles and also the two most stable surfaces of Fe, (111) and (110), were studied by characterizing the type of interaction present between the substrates and the adsorbates. Arsenic acid (H_3AsO_4) is spontaneously reduced in both extended surfaces of iron, producing arsenious acid and oxidizing the metal surface. Arsenious acid (H_3AsO_3) completely decomposes into (AsOH)(OH)(OH) fragments on the smallest particles, Fe_{32} and Fe_{59}, but also on the (111) surface. However, on greater particles (NP_{80} and NP_{113}) and on the (110) surface, H_3AsO_3 retains its initial free configuration and is joined to the surface through both atoms, As and O. Large dispersion components of the adsorption energy were observed when the acids interact with the substrates without decomposition. From a Bader analysis of the atomic charges, important charge transfers were found. Both the As and the interacting Fe atom are slightly reduced on the (110) surface and NP_{80}. However, the four nearest neighboring irons are oxidized because of the interaction with H_3AsO_3. In the case of the Fe_{32} cluster, where this acid is totally broken, all the interacting Fe atoms are oxidized. A significant decrease of the magnetic moment was found for the Fe atom that interacts with H_3AsO_3. This fact was confirmed with the diminution of the spin