

# First principles study about Fe adsorption on planar SiC nanostructures: Monolayer and nanoribbon



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## ABSTRACT

Spin polarized density functional theory (SP-DFT) has been used to investigate the stability and electronic properties of Fe adsorption on SiC, both monolayer and nanoribbon (NR). For the monolayer, we obtain a magnetic moment of  $2 \mu_B$  ( $6 \mu_B$ ) when an Fe atom (dimer) is adsorbed on top of a hexagon. The Fe adsorption gives rise to new electronic levels inside the band gap. Fe atoms and dimers are preferentially adsorbed on top of the hexagon center of the NR, which is localized at the border of the NR. Afterwards, new electronic properties of Fe adsorption are observed for the NR. For an isolated Fe atom to be adsorbed the system must be semiconductor with different band gaps for the two spin channels; however, for an Fe dimer to be adsorbed, we must obtain a spin gapless semiconductor (SGS). When the two borders of the SiC nanoribbon are equally drawn with Fe atoms, two magnetic states are obtained, which is dependent upon the edge coupling. The ferromagnetic (FM) is the most stable state and half-metallic properties are shown while for the antiferromagnetic (AFM) a narrow band gap semiconductor is obtained.

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## 1. Introduction

Although Si and C are located in the same column of the periodic table, they show different electronic properties. This happens because C prefers the  $sp^2$  hybridization while Si prefers the  $sp^3$  hybridization. Silicon carbide (SiC) is a binary compound with Si and C in the 1:1 stoichiometry, which can crystallize in many different structures. The best known is the cubic (3C-SiC), hexagonal (2H-SiC, 4H-SiC and 6H-SiC) and the rhombohedra (15R-SiC and 21R-SiC). This wide band gap semiconductor has high-saturated electron mobility and high thermal mobility and is thus suitable for harsh environments such as those with high temperature, high pressure, high frequency [1]. Low dimensional SiC nanostructures, like nanotubes (NTs) and nanowires (NWs), have been synthesized and have prompted interest due to their novel properties. For example, SiC NTs are always semiconductors, independent of their diameter and chirality.

Recently, C arranged in a two-dimensional single hexagonal atomic layer with  $sp^2$  hybridization (graphene) has been synthesized [2]. These two-dimensional structures have unique electrical and mechanical properties, which have never been observed in conventional three-dimensional materials. By cutting graphene in ribbons, we obtain graphene nanoribbons (GNRs), which present

electronic properties dependent on the edge termination. The GNRs terminated by H atoms with armchair borders are nonmagnetic semiconductors, while the GNRs terminated with H atoms that have zigzag borders are magnetic and can be metallic (FM interaction between the borders) or semiconductors (AFM interaction between the borders) [3].

SiC NTs and SiC NWs are nonmagnetic semiconductors with large band gaps [4]. However the presence of defects could give rise to new magnetic and electronic properties [5–7]. Similar to C, SiC is able to form planar nanostructures arranged in two (layers) and one dimension (ribbons) [7–10]. Electronic and magnetic properties of SiC nanoribbons (SiCNRs) depend upon edge termination. The SiCNRs with H termination (H-SiCNRs) and armchair termination are nonmagnetic semiconductor, while the H-SiCNRs with zigzag termination are magnetic and can be metallic, half metallic or semiconductor depending on ribbon width and magnetic coupling [11]. The new electronic properties shown by the SiCNRs allow the usage of SiCNRs in spintronics.

To optimize metal contact in the development of devices based on SiC nanostructures, a study about the stability and electronic and magnetic properties of metal adsorption on planar SiC nanostructures is necessary. Fe is the most common and cheapest metal on earth and has a magnetic ground state. In order to functionalize the planar nanostructures, the adsorption of atomic Fe and also Fe dimer on graphene and GNRs have been intensely studied using first principles studies [13–24]. These doped nanostructures

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presented new electronic and magnetic properties, which increase the possibility of using the planar structure in many applications, such as charge transport, spintronics and hydrogen storage. In order to investigate the possibility of creating and manipulating a spin current polarized in planar SiC (monolayer and NR), we use first principles calculations within the SP-DFT to analyze the interaction between Fe (atoms and dimers) and a planar SiC nanostructure. Our results show that Fe is strongly and preferentially adsorbed on top of an SiC ring. Fe atoms and dimers are preferentially (most stable site) adsorbed at the border of the NR and give rise to different magnetic and electronic properties to the SiCNRs. When the borders of the SiCNRs are equally appointed with Fe atoms, two magnetic states can be observed, depending on the magnetic coupling between the borders. The FM (most stable) is a half-metallic system while the AFM is a narrow band gap semiconductor.

## 2. Methodology

The calculations are performed within the SP-DFT framework and for the exchange–correlation term the generalized gradient approximation (GGA) [25] is used. The Kohn–Sham (KS) equations are solved using the self-consistent method, as implemented in the Vienna *ab initio* simulation package (VASP) [26,27]. The valence electrons and the ionic core interactions are described through the PAW method [28]. The KS orbitals are expanded in a plane wave basis set with an energy cutoff of 400 eV. It is known that GGA is not able to properly describe the d sub bands from the Fe atom. The use of GGA + U approximation (U is an empirical orbital term, which comes from the Hubbard Hamiltonian) improve the DFT and magnetic moments predicted can be obtained by DFT calculations only when the U term is used, as was observed for Fe interaction with a vacancy in graphene [29]. In our calculations we opted to not use the U term, it is justified when the results are discussed.

We use the supercell approach and both monolayer and NRs are studied in the 1:1 stoichiometry. In the monolayer, all C (Si) atoms have three Si (C) as nearest neighbor while, in the NR, the C (Si) bonds at the border of the NR termination are saturated by H atoms. In the monolayer, the dimensions of the supercell are 19.55 Å and 16.87 Å (Fig. 1(a)), while the supercell for the NR is a (7,7) zigzag aligned along the X direction and has dimensions of 12.56 Å and 31.40 Å along the X and Y directions, in respective order. To ensure negligible interactions between images, a vacuum region of 10.0 Å was used along the Z direction. To ensure

non-interaction between the NRs borders the supercell has a vacuum of about 10.0 Å along the Y direction.

To sample the Brillouin zone and calculate periodic functions, a  $5 \times 5 \times 1$  and a  $21 \times 1 \times 1$  Monkhorst–Pack grid were used to generate the special k-point for the monolayer and NR, respectively. All the atoms in the supercell are allowed to relax without imposing any symmetry constraint. The forces are calculated using the Hellmann–Feymann procedure and the geometries are optimized using the conjugated gradient (CG) method. The system is relaxed until the root mean square criterion of 0.04 eV/Å on the atomic forces is reached.

We calculate the adsorption energy ( $E_{\text{ads}}$ ) for each adsorbed Fe atom (dimer) using total energy calculations, according to the equation:

$$E_{\text{ads}}[\text{Fe}]/n = \{E_{\text{T}}[\text{pristine}] + n\mu_{\text{Fe}} - E_{\text{T}}[n\text{Fe}]\}. \quad (1)$$

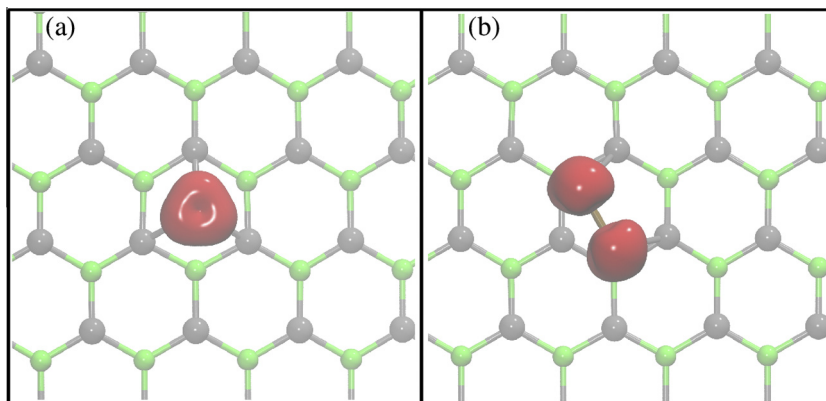
In Eq. (1),  $E_{\text{T}}[n\text{Fe}]$  is the total energy of the supercell with  $n$  adsorbed Fe atoms (dimers),  $E_{\text{T}}[\text{pristine}]$  is the total energy of the pristine system, and  $\mu_{\text{Fe}}$  is the total energy of an isolated Fe atom (dimer). Positive values of  $E_{\text{ads}}$  indicate that Fe atoms (dimers) are readily adsorbed (an exothermic process).

## 3. Results and discussion

Initially, we calculate the electronic band structure for pristine systems. Our results are in accordance with previous theoretical calculations [12]. We obtain that the monolayer is a wide band gap semiconductor with no spin splitting. Two magnetic states can be obtained for the NR. The ground state is a narrow band gap semiconductor and the magnetic coupling between the borders is AFM, while the FM coupling has higher energy ( $\approx 50$  meV) and metallic characteristics are observed.

Next, we look for the most stable configuration for the adsorption of a unique Fe atom per supercell in the SiC monolayer. The Fe atom is adsorbed on top of a hexagon center with adsorption energy of 2.46 eV, being 0.54 eV higher than that obtained by Bekaroglu et al. [30]. After the Fe adsorption, a spin magnetic moment of  $2 \mu_{\text{B}}$  ( $\mu_{\text{B}}$  is the Bohr magneton) is present and localized in the Fe atom, as shown in Fig. 1(a). It is noteworthy that our results for the magnetic moment are in accordance with previous first principles calculations of the Fe atomic adsorption on a SiC monolayer [30].

In Fig. 2, we show the electronic band structure of the SiC monolayer, before 2(a) and after 2(b), the Fe atomic adsorption. As can be noticed, the Fe atom introduces four electronic levels



**Fig. 1.** Local geometric configuration and the electronic charge density (pup–pdown), in red, when an (a) Fe atom or (b) dimer is adsorbed per unit cell on an SiC monolayer. Small green, gray and ochre balls represent the C, Si and Fe atoms, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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