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# DFT calculations of graphene monolayer in presence of Fe dopant and vacancy

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ABSTRACT

In the present work, the effects of Fe doping and vacancies on the electronic, magnetic and optical properties of graphene are studied by density functional theory based calculations. The conductive behavior is revealed for the various defected graphene by means of electronic density of states. However, defected structures show different magnetic and optical properties compared to those of pure one. The ferromagnetic phase is the most probable phase by substituting Fe atoms and vacancies at AA sublattice of graphene. The optical properties of impure graphene differ from pure graphene under illumination with parallel polarization of electric field, whereas for perpendicular polarization it remains unchanged. In presence of defect and under parallel polarization of light, the static dielectric constant rises strongly and the maximum peak of Im $\varepsilon(\omega)$ shows red shift relative to pure graphene. Moreover, the maximum absorption peak gets broaden in the visible to infrared region at the same condition and the magnitude and related energy of peaks shift to higher value in the EELS spectra. Furthermore, the results show that the maximum values of refractive index and reflectivity spectra increase rapidly and represent the red and blue shifts; respectively. Generally; substituting the C atom with Fe has more effect on magnetic and optical properties relative to the C vacancies.

## 1. Introduction

Recently, spintronics has become one of the new branches in electronics. The aim in spintronics is transferring more information with the less energy consumption. Regarding that, magnetic materials with high conductance are needed to use as electrodes in spintronics devices. On the other hand, graphene has attracted the attention of researchers increasingly because of its wonderful properties such as high transparency [1], extremely high mobility [2,3], zero dark current when used as photosensitive devices [5], spin relaxation length more than 1.5 μm [4], and etc. Therefore, at the first glance, graphene is a suitable material for use in optoelectronic applications like optical gas sensor [6,7], solar cells [8,9], LEDs [10,11], photodetectors [12,13]. However the non-magnetic behavior of pure graphene (G) leads it to be inappropriate for spintronics. Hence, different methods are suggested to overcome this problem such as: tailoring of graphene to zigzag nanoribbons [14], deposition of magnetic layer on the graphene surface [15], defect creation in the crystal structure of graphene such as vacancies [16] and substituting carbon atoms with the *d*-type transition metals [17]. The latest method is a good way in the low concentration of defects that also keeps the metallic behavior of graphene. In fact, the difference between spin-up and spin-down band gap energy of graphene doped with transitional metals such as Fe, Co and Ni promotes its application in spintronic field [18]. Additionally, the composite of Fe on graphene substrate can act as a possible Pt-free alternative catalyst for fuel cells [19]. Moreover, it is predicted that Fe doped graphene with a low cost and environmental friendly behavior is a highly stable adsorbent [20,21]. Researchers have shown that Fe doped graphene could be a promising candidate for sensing Nitrogen Oxides and $H_2CO$ [22,23].

Basically, two different sublattices A and B are introduced in graphene (Fig. 1a). Researchers have shown that the presence of the magnetic atoms in the same (AA or BB) and different sublattices (AB) results in a ferromagnetic (FM) and anti-ferromagnetic (AFM) order, respectively [24,25].

Regarding this magnetic behavior and the particular optical properties of graphene, it can be one of the candidates for spin-optoelectronics [26]. Spin-optoelectronics involves interaction of light with electrons considering their spin effect, which are investigated recently. In order to have better envision related to the spin-optoelectronic devices based on the graphene, the magnetic and optical properties of that should be

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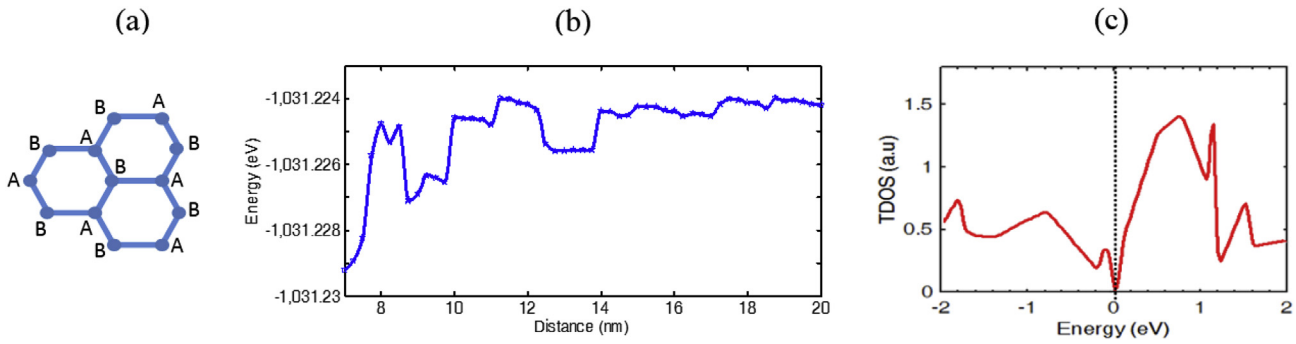


**Fig. 1.** (a) Schematic of graphene with its sublattices, (b) energy changes versus the interlayer separation of graphite, (c) the total electronic density of state (TDOS) versus the energy for pure graphene.

discussed.

In this paper, the effect of Fe impurities and vacancies on the magnetic and optical properties of graphene and the connection between them is investigated. The rest of the article is organized as follows. In Section 2 the detailed computational method used for computing the desired properties has discussed. Section 3 covers the results related to the obtained electronic, magnetic and optical properties and their relations. Finally, conclusions on this computational work have been drawn in Section 4.

## 2. The methodology

Density functional theory (DFT) is one of the most accurate methods to identity the solid specifications. Here, the full linear augmented plane wave (FLAPW) method based on DFT as embodied in *ab* initio WIEN2k code [27] is used to calculate the electronic, magnetic and optical properties of the graphene structure. In the FLAPW method, the unit cell is divided into non-overlapping ("muffin tin") sphere with radius $R_i$ and an interstitial region. Exchange and correlation effects, the unknown segment in DFT method, were treated within the generalized gradient approximation (GGA) using the scheme of Perdew–Burke–Ernzerhof (PBE) [28,29].

The parameter $R_{K\max} = R_{mt} \times K_{\max}$, which controls the size of the basis set in these calculations, was chosen 6 ($R_{mt}$ is the smallest muffin tin radius and $K_{max}$ the largest wave number of the basis set) and the first Brillouin zone integration in the *k*-space was done by 1000 *k*-points for every unit cell. The threshold on energy, charge, and force was set to $10^{-4}$ eV, $10^{-3}$ electrons per atom, and $10^{-3}$ Ry/a.u., respectively during the self-consistent process.

To simulate the graphene layer, the graphite crystalline structure (P6/mmm, $a = b = 2.45A^{\circ}$, $c = 6.69A^{\circ}$, $\alpha = \beta = 90^{\circ}$, $\lambda = 120^{\circ}$) was considered firstly. Then to avoid the interaction between two carbon layers in graphite structure, the interlayer separation was increased until the energy changes converted to desired value (less than 0.001 eV). So with

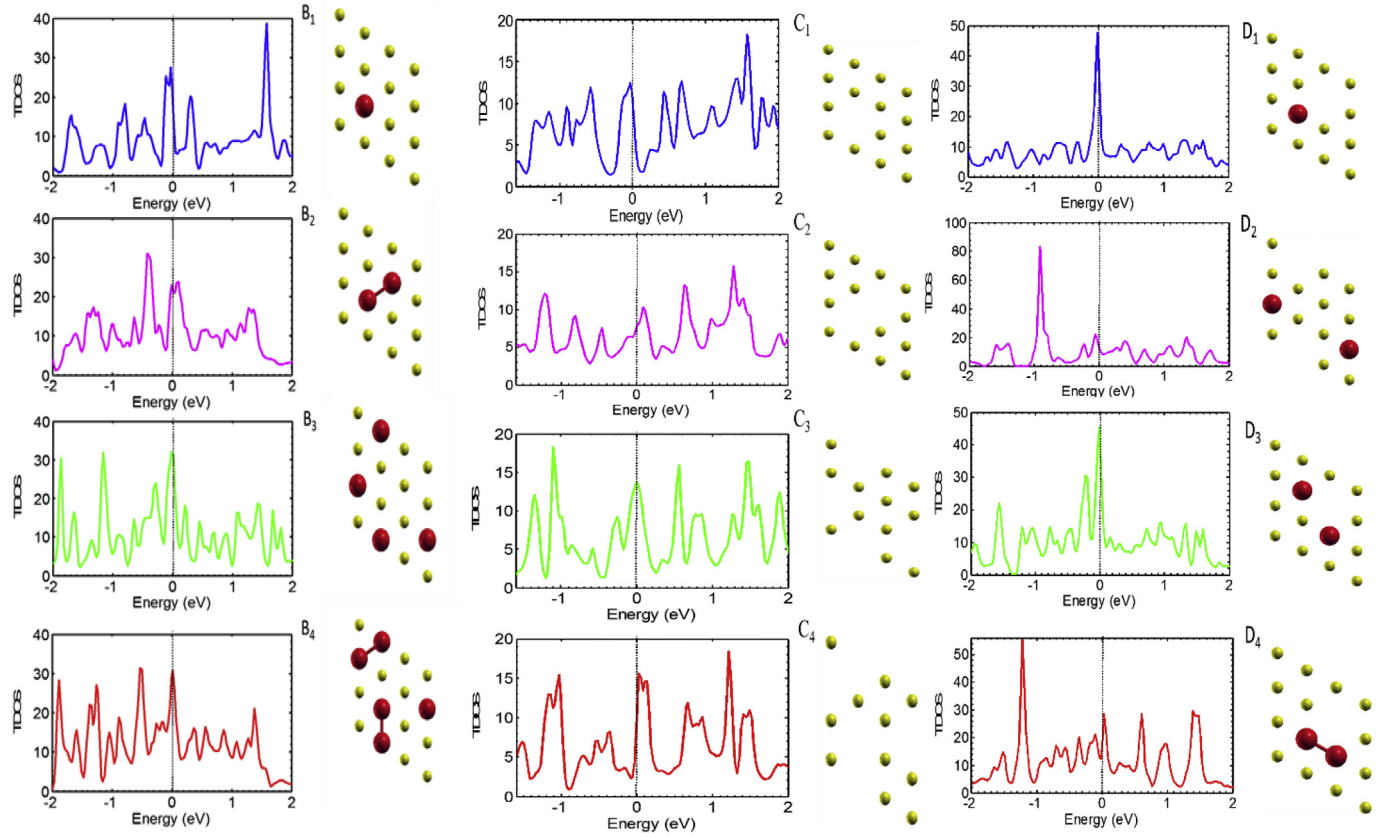


**Fig. 2.** The supercell structure of different defected graphene and TDOS curves versus the energy for them.