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# Effect of doping of graphene structure: A Monte Carlo simulations

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ABSTRACT

In this work, we have studied the effect of magnetic atom doping of graphene structure using Monte Carlo simulation. The reduced critical temperature with the magnetic atom doping $x$ has been deduced from the thermal variation of magnetization and magnetic susceptibility. The variation of magnetization versus the crystal field of grapheme structure for different $x$ and for different reduced temperatures has been established. We also have measured the coercive field ($h_C$) as a function $x$ in grapheme structure, finding that $h_C$ increases with increasing $x$ concentration as predicted experimentally. The doping-induced magnetism in graphene. Magnetically atom doping in graphene systems are potential candidates for application in future spintronic devices, magnetometry requires macroscopic quantities of graphene to detect magnetic moments directly.



## 1. Introduction

Carbon is a unique nonmagnetic element due to its considerable features [1]. Among the carbon allotropes, graphene nanoribbons have attracted more attention than other structures due to their edge state and width [2]. Magnetic materials and nanostructures based on carbon offer unique opportunities for future technological applications such as spintronics [3]. Despite theoretical advances in the study of nanoribbons, and some recent experimental results hinting at signatures of this edge magnetism [4], the difficulty in patterning the edge geometries required for these effects to be observed may prevent a wider scale exploitation. Another possibility that has been proposed for graphene-based spintronics is the exploitation of vacancy-driven magnetic moments that arise in graphene [5–7]. A dilute distribution of magnetic impurities is assumed to be present in doped graphene [8]. Kinetic lattice Monte Carlo simulations, implementing *ab initio* calibrated energetics, are applied to study the evolution of vacancy systems in graphene [9]. The analysis of the total density of states and partial density of states indicates that the magnetic properties of doped graphene originate from the p–d exchange, and the magnetism is given a simple quantum explanation using the Ruderman–Kittel–Kasuya–Yosida exchange theory [10]. The mean-field approach, of the kinetics of a mixed ferrimagnetic model on a square lattice in which two interpenetrating square

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sublattices have spins that can take two values, s = ±1/2, alternated with spins that can take the four values, S = ±3/2; ±1/2 is studied [11]. In previously works [12–14] the thermodynamic properties of a nano-graphene bilayer, consisting of the upper layer A of spin-3/2 with antiferromagnetic intralayer exchange coupling and the bottom layer B of spin-5/2 with ferromagnetic intralayer exchange coupling, have been studied by the use of Monte Carlo simulation. Monte Carlo method is used to investigate the phase diagram of the ferromagnetic two-dimensional mixed spin-1 and spin-1/2 Ising model with four-spin interaction $J_4$ and next-nearest couplings J' [15]. The phase transition properties of Ising, classical XY and Heisenberg of diluted ferromagnetic thin film are studied by the method of exact high-temperature series expansions extrapolated with the Padé approximants method [16]. The Introduction is presented in section 1. The theory and model are established in section 2. The Monte Carlo simulations has been given in section 3. The Results and discussion have been given in section 4. Finally, we have given the conclusion in section 5.

## 2. Theory and model

In previous work [17] the system of spin-1/2 magnetic impurities distributed over two-dimensional hexagonal lattice sites in on-site positions is investigated. In this work, we have used a graphene structure constituted by non-atom magnetic and magnetic atom doping with spin-2, as depicted in Fig. 1 and such as $Fe^{2+}$, $Co^{3+}$,$Cr^{2+}$ or $Mn^{3+}$. The Hamiltonian used it is includes first and second nearest neighbors interactions, the crystal field and external magnetic field and is given as:

$$H = -\frac{J_1}{J_2}\sum_{<i,j>}\eta_i\eta_j S_i S_j - \sum_{<<i,k>>}\eta_i\eta_k S_i S_k - \frac{\Delta}{J_2}\sum_i \eta_i S_i^2 - \frac{h}{J_2}\sum_i \eta_i S_i \quad (1)$$

where $\langle i,j\rangle$ and $\langle\langle i,k\rangle\rangle$ stand for the first nearest neighbor sites ($i$ and $j$) and the second next nearest neighbor interaction ($i$ and $k$), respectively, $\Delta$ represent the crystal field and $h$ is the external magnetic field. Where η variables can have the values 0 or 1 depending on whether the magnetic site i(j or k) exists or not. The $J_1$, and $J_2$ are the exchange interactions between magnetic atom with magnetic spins moment ($S_i$-$S_j$) and ($S_i$-$S_k$) such as given in Fig. 1. The spin moments of $S_i$ are: S = ±2;±1;0. The new parameter used in full text is: $R = J_1/J_2$.

## 3. Monte Carlo simulations

The graphene systems constituted by the nonmagnetic atom $N_S$ = 200 and magnetic atom doping with spin-2 and concentration, $x$ varying between 0 and 1. We apply a standard sampling method to simulate the Hamiltonian given by Eq. (1). Cyclic boundary conditions in the (x,y) plane on the lattice were imposed and the configurations were generated by sequentially traversing the lattice and making single-spin flip attempts. The flips are accepted or rejected according to a heat-bath algorithm under the Metropolis approximation (see chart of Monte Carlo simulations).

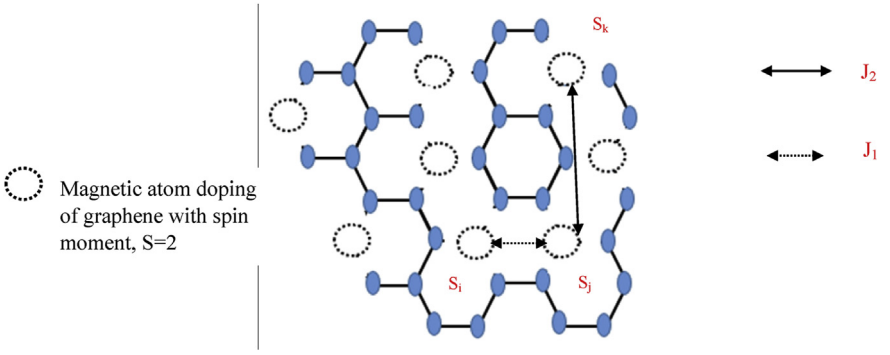


**Fig. 1.** Schematic illustration of two substitutional the non magnetic atom (blue circles) embedded in a graphene lattice and dotted circles are the magnetic atoms with spin moment S = 2 such as $Fe^{2+}$, $Co^{3+}$,$Cr^{2+}$ or $Mn^{3+}$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)