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Size and diluted magnetic properties of diamond shaped graphene quantum dots: Monte Carlo study

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HIGHLIGHTS

- Magnetic properties of diamond shaped graphene quantum dots have been investigated.
- Magnetizations and magnetic susceptibilities have been calculated.
- Effect of exchanges interactions and crystal field on magnetization has been given.
- Magnetic hysteresis have been obtained for diamond shaped graphene quantum dots.
- Magnetic coercive increases with increasing the exchange interactions.
- Magnetic coercive decreases when the temperatures values increasing.

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ABSTRACT

The magnetic properties of diamond shaped graphene quantum dots have been investigated by varying their sizes with the Monte Carlo simulation. The magnetizations and magnetic susceptibilities have been studied with dilutions x (magnetic atom), several sizes L (carbon atom) and exchange interaction J between the magnetic atoms. The all magnetic susceptibilities have been situated at the transitions temperatures of each parameters. The obtained values increase when increases the values of x, L and J. The effect of exchanges interactions and crystal field on the magnetization has been discussed. The magnetic hysteresis cycles for several dilutions x, sizes L, exchange interactions J and temperatures T. The magnetic coercive increases with increasing the exchange interactions and decreases when the temperatures values increasing.

1. Introduction

In recent years, magnetic, graphene, single layer of graphite with excellent conductivity has stimulated the interest of scientists due to the possibilities of several applications in the field of nano-electronics [1,2], graphene based polymer nanocomposites [3–5] and graphene quantum dots [6]. In other hand, the graphene–diamond hybrids have recently attracted researchers to theoretical predictions of the interface between the two allotropes and their electronic properties, using ab initio density functional calculations [7–9], effective field theory [10] and experimentally [11]. Graphene under a uniform magnetic field described by the two-dimensional Dirac oscillator model is discussed based on the approach of the effective mass and the zeta function. Thermodynamic properties of graphene, such as the free energy, the mean energy, the entropy and the specific heat have been found [12]. Vacancy defects in single-layer graphene and silicene exhibit unusual interesting

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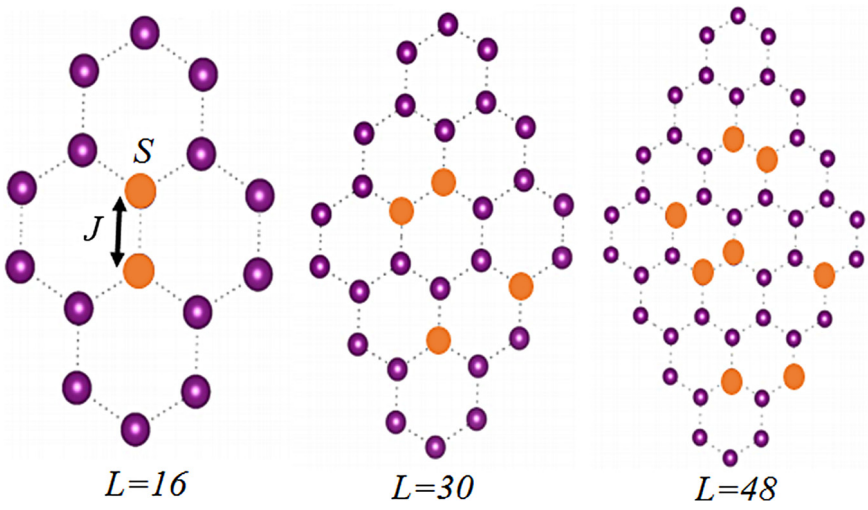

Fig. 1. Different structures with several size $L = 16$, 30, and 48 carbon atoms respectively from left to right.

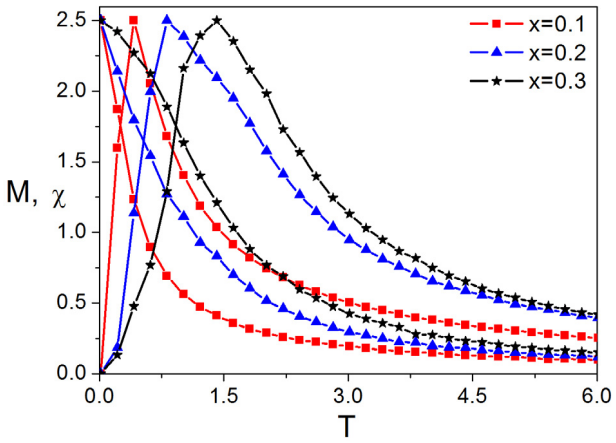

Fig. 2. The magnetizations and magnetic susceptibilities with dilution $x = 0.1, 0.2, 0.3$ for $J = 1.0$ K, $\Delta = 0.0$, $h = 0.2$ T and $L = 48$.

electronic and magnetic properties [13] emerging from their honeycomb structures and rotation symmetries. Recently, we have demonstrated [14] the magnetism of silicene under mono-vacancy, divacancy and substituted atoms such as Al and P. In other hand the energetic stability, electronic, and magnetic properties of hydrogenated graphene nanoflakes using density-functional theory are also studied [15]. We note that in addition of the effect of crystal structural, the magnetic anisotropy can also depend on the size of the nano-crystals [16]. The effects of edge disorder and roughness for graphene nanoribbons in relation to their armchair or zigzag orientation is also studied [17]. Magnetic properties of the main allotropic modifications of carbon (diamond, graphite, nanographite, nanotubes, fullerenes) are described [18] and the magnetic properties of nanoparticle, nanoisland, nanoribbon, metallic nanotube and nanowire are studied with Ising model [19–24]. In a magnetic field, these edge states, strongly localized near zigzag edges, generate a rational fraction of the magnetic flux in each hexagon, and thus behave like zero-field edge states [25]. Furthermore, defective zigzag graphene nanoribbons structures show magnetic moment by supercell up to 2.0 μ_B [26]. The Ni nanotubes and nanowires with an average diameter of about 140 nm are synthesized by a template-assisted sol–gel autocombustion method using nickel nitrate, citric acid and ammonia as the starting materials [27]. The effect of transition metal atoms on the magnetic properties of nano, bilayer and trilayers-graphene, have been systematically studied by effective-field theory and first principles calculations [28–31]. The behavior of ground state phase diagrams of a mixed Ising spins model on a bipartite square lattice of spins-2 and 5/2 have been also investigated [32]. This the mixed spin-2 and spin-5/2 Ising ferrimagnetic system is used on a layered honeycomb lattice in which Fe^{II} ($S = 5/2$) and Fe^{III} ($\sigma = 2$) occupy sites [33]. In this paper, the diamond shaped graphene quantum dots Ising model with the single-ion anisotropy is suggested in Fig. 1. The system is formed with diamond shaped graphene quantum dots constituted with carbon atoms diluted by magnetic ion with spin $S = 5/2$ such as Sm^{3+}, Dy^{3+}, Mn^{2+}, Fe^{3+}