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Study Of Magnetic Moment of Nano Structured Functionalized Graphene Within DFT Calculations

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ABSTRACT : Nano systems show a wide variety of change in their properties, magnetic properties are no exception. In this paper we look at how magnetic properties of graphene change on functionalization with hydrogen. This material has emerged as an amazing material for microelectronic devices. Calculations based on the method of numeric localized atomic orbitals, pseudopotentials and DFT are presented using SIESTA code for the systematic study of Magnetic Moment of nano structured functionalized graphene. It has been observed that as the percentage of hydrogen increases, a variation in the magnetic moment takes place pointing to a transition of of nano structured functionalized graphene from diamagnetic to paramagnetic/ferromagnetic phase with varying percentage of hydrogen.

Keywords: Graphene, DFT, SIESTA, Magnetic Moment.

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1. INTRODUCTION

Graphene, which was isolated from graphite 440 years after the invention of pencil, represents a new class of materials which are only one atom thick. It offers new inroads in to low dimensional properties and continues to provide fertile ground for applications. Particularly functionalized graphene has emerged as an amazing material for microelectronic devices [1-7]. We have undertaken a study of nano structured functionalized graphene modelled in chair conformation having 18 carbon atoms with varying concentrations of hydrogen atoms. The number of hydrogen atoms were increased from 0 to 18 as shown in Fig. 1 (*a*) and (*b*) for pure graphene and functionalised graphene respectively. In all nineteen systems have been studied.

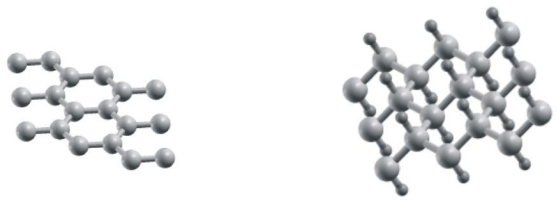

Fig. 1. (A) Nano Structured Graphene (18C atoms) (B) Funtionalized Graphene (18C + 18H atoms) in Chair onformation.

II. SIMULATION DETAILS

Calculations are based on the method of numerical localized atomic orbitals, pseudopotential and DFT using SIESTA code siesta-3.0–*b* version [8, 9]. We have used Troullier Martin, norm conserving, relativistic pseudopotentials in fully separable Kleinman and Bylander form for both carbon and hydrogen. The exchange and correlation energies are treated within the generalized gradient approximation (GGA) according to the Perdew, Burke, Ernzerhof (PBE) parameterization.

The used pseudopotentials were tested for properties of molecules such as CH_4 providing us converged parameters for the present study. Throughout geometry optimization, numerical atomic orbitals with double zeta polarization (DZP) basis set with confinement energy of 0.01 Ry were used. 11 × 11 × 1 Monkhorst-Pack of k points was used for sampling Brillouin zone. The spacing of the real space grid used to calculate the Hartree and exchange and correlation contribution to the total energy and Hamiltonian was 450 Ry. The exchange correlation functional used was PBE authored by Perdew, Burke, Ernzerhof. Minimization of energy was carried out by giving sufficient number of SCF iterations using standard conjugate-gradients technique [9].

III. RESULTS AND DISCUSSION

Magnetic moment has been calculated using SIESTA code for nano structured functionalized graphene varying the no. of H atoms from 0 to 18 in the chair conformation. In all, 19 structures have been studied. The results are shown in Table 1 and Fig. 2. First graph from top in Fig. 2 shows the variation of magnetic moment when no. of H atoms are even (green line) and when the no. of H atoms are odd (red line). In the second graph from top, *n* is even and varies from 0 to 10. In the third graph from top, *n* is even and varies from 10 to 18. In the fourth graph from top, n is odd and varies from 1 to 17.

Table 1: Variation of Magnetic Moment of Functionalized Graphene with H atoms in chair conformation.

No. of H atoms (Even)	Magnetic Moment(μ_B)	No. of H atoms (Odd)	Magnetic Moment(μ_B)
0	0.000375	1	1.000129
2	–0.000444	3	0.999964
4	0.000409	5	0.999999
6	0.024144	7	0.999999
8	–0.000424	9	1.000000
10	–0.000000	11	1.000001
12	1.990303	13	0.999999
14	–0.000656	15	1.000002
16	2.000000	17	0.999993
18	0.000000		

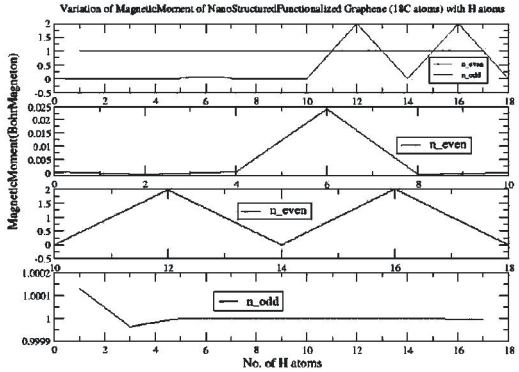

Fig. 2 Variation of Magnetic moment of nano structured functionalized graphene with no. of H atoms in chair conformation.

Fig. 2 shows the variation of magnetic moment. with the no. of H atoms. As the number of H atoms are increased fron 0 to 18 in chair conformation, a variation in the magnetic moment is observed. Pure graphene has a magnetic moment of 0.000375. When *n* is odd, the magnetic moment varies between 1.000129 (for n = 1) to 0.999993 (for n = 17). When n is even, the magnetic moment varies from 0.000656 (for n = 14) through 0.000000 (n = 10 and 18) to 2.000000 (for n = 16).

Thus, with the variation of percentage of *H* atoms, the functionalized graphene shows a variation in the magnetic bahaviour from diamgnetic, for very low values of magnetic moment to paramagnetic/ferromagnetic for substantial value of magnetic moment. This property is useful for the applications of functionalized graphene in microelectronics.

IV. ACKNOWLEDGEMENT

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