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AB INITIO STUDY OF NANO STRUCTURED FUNCTIONALIZED GRAPHENE WITH 30C ATOMS

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Abstract: We have studied the electron density of states and formation energy for nano structured functionalized graphene with 30C atoms. Our calculations are based on the method of numeric localized atomic orbitals, pseudopotentials and DFT using SIESTA code. As the no. of hydrogen atoms increases from 1 to 30, variation in the forbidden energy gap appears near the Fermi energy and behaviour of nanostructure changes from conductor to semiconductor/insulator. The formation energy is found to increase linearly as the no. of hydrogen atoms increases, indicated that functionalized graphene is more stable.
Keywords: Graphene, DFT, SIESTA, Electronic Density of States.
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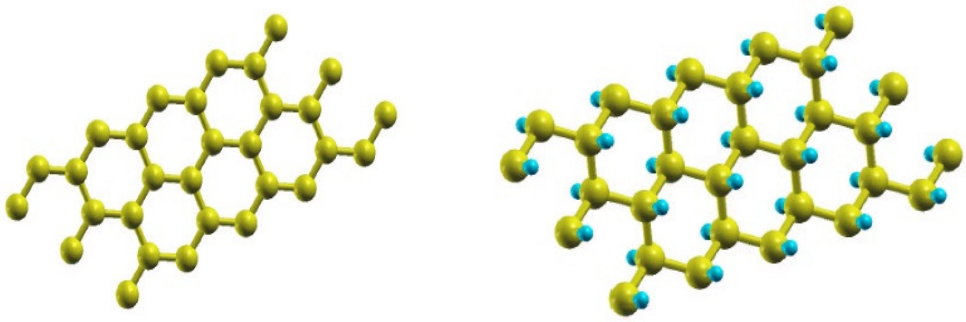
1. INTRODUCTION

Graphene, a single hexagonal atomic sheet of carbon atoms from bulk graphite, has attracted immense interest due to its fascinating electronic properties [1-6]. Its unusual basic properties [3] motivated significant research efforts. It has the potential for a large number of applications in microelectronics, optoelectronics and for hydrogen storage. Functionalized graphene has emerged as an amazing material for microelectronic devices [7-10]. It is possible to change the electronic properties of graphene by chemical functionalization so that it can be more useful for applications in nanoelectronics.

In this work we study a nanostructure of functionalized graphene modeled in chair conformation having 30 carbon atoms with varying concentration of hydrogen atoms. The no. of hydrogen atoms is increased one by one from 1 to 30. The optimised structures and electron density of states (DOS) has been obtained for 31 nanostructures. Fig. 1(a & b) shows the optimised structures for 30C (pristine graphene) and 30C+30H (fully functionalized graphene in chair conformation). Our calculations are performed within density functional theory as implemented in SIESTA code [11, 12].



(a) **(b)**

Fig.1 Optimised structures (a) Graphene with 30C atoms (b) Functionalized Graphene with 30C+30H atoms in chair conformation.

2. Simulation details

Calculations are based on the method of numeric localized atomic orbitals, pseudopotential and DFT using SIESTA code siesta-3.0-b version [11, 12]. 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 local density approximation (LDA) according to the Ceperlay Alder (CA) 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 0.02 Ry were used. A 6x6x1 Monkhorst-Pack of k points was used for sampling Brillouin zone. The spacing of the real space grid used to calculate the Hartree, exchange and correlation contribution to the total energy and Hamiltonian was 250 Ry. The exchange correlation functional used was LDA authored by Pedrew and Zunger. Minimization of energy was carried out by giving sufficient number of SCF iterations using standard conjugate-gradients technique [12].

3. Results and Discussion

The results of the simulation are shown in Fig. 2 and Fig. 3. As the no. of hydrogen atoms is increases from 1 to 30 one by one placed in the chair conformation, variation in energy gap appears near the Fermi energy. Fig.2 shows the results for pure graphene (Fig.2a) and for functionalized graphene [Fig.2 (b-d)]. When the no. of hydrogen atoms is odd a peak appears at the Fermi energy indicating the nano structure is a conductor

(Fig.2b). When the no. of hydrogen atoms is 14 & 16, a small forbidden energy gap appears near the Fermi energy indicating that these nanostructures behave as semiconductors. When the no. of hydrogen atoms is 8, 12, 18, 20, 22, 26, 28 and 30 a large forbidden energy gap appears near the Fermi energy indicating that these nanostructures are insulators (Fig.2c and 2d). When the no. of hydrogen atoms is 10 & 24 there is no forbidden gap near the fermi energy and these nanostructures behave as conductors.

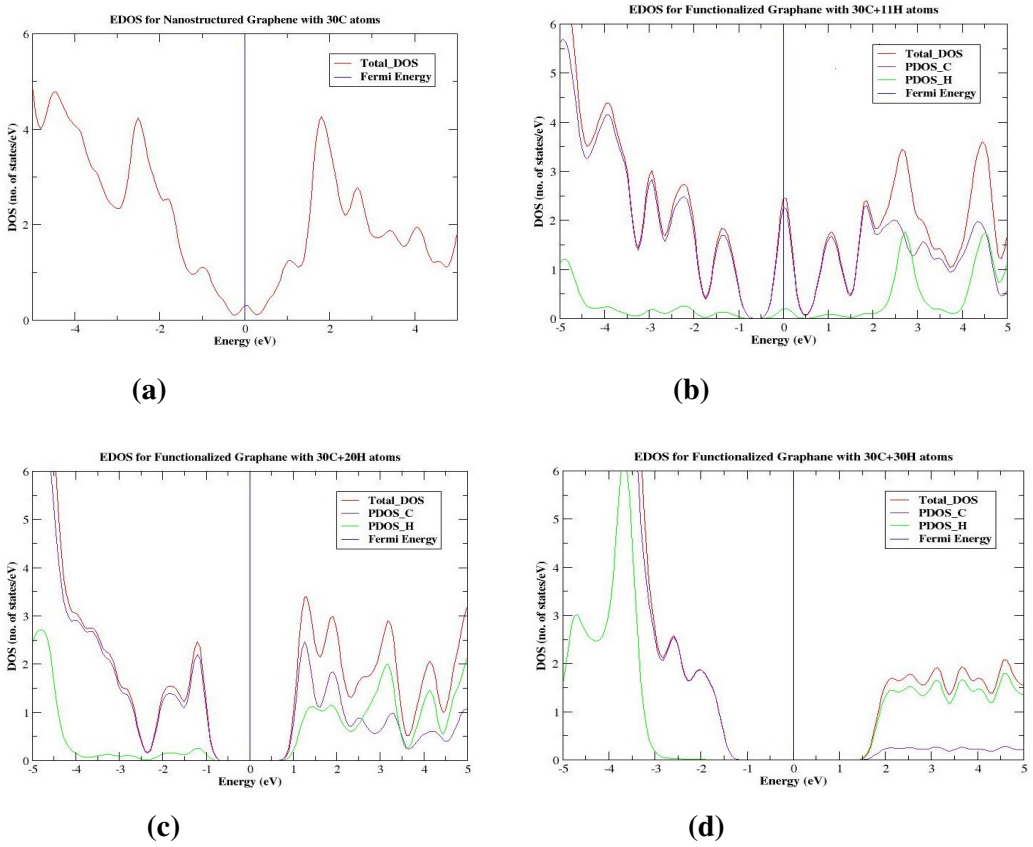


Fig.2 Graph of Total DOS and projected DOS for (a) Graphene with 30C atoms (b) Functionalized Graphene with 30C+11H atoms (c) Functionalized Graphene with 30C+20H atoms (d) Functionalized Graphene with 30C+30H atoms (The zero of the energy scale lies at the Fermi energy).

The formation energy E_s of the functionalized graphene was calculated using the formula

$$E_s = E_T - N_c E_c - N_H E_H \qquad (1)$$

Where E_T is the total energy of the functionalised graphene, E_c total energy of the single carbon atom and E_H the total energy of the single hydrogen atom obtained from converged SIESTA runs.

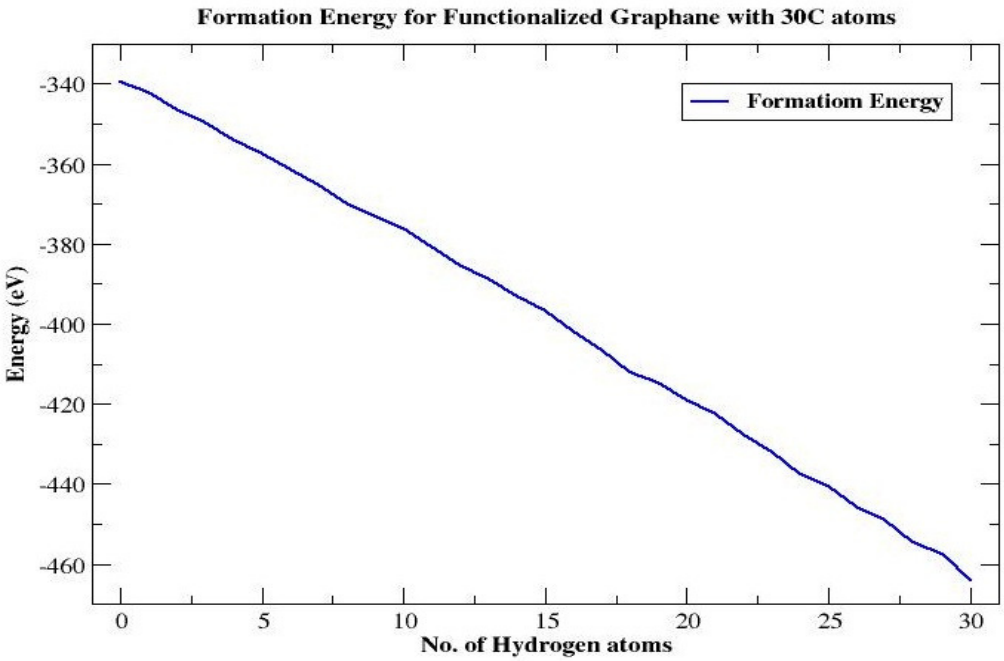


Fig.3 Graph of variation in Formation Energy of functionalized graphene as the no. of hydrogen atoms is increased.

In Fig.3 formation energy has been plotted against the no. of hydrogen atoms for all 31 nanostructures. The formation energy increases almost linearly as the number of hydrogen atoms increases, indicating that functionalized graphene is more stable.

4. Conclusion

Our simulation reveals that on hydrogenation a forbidden energy gap appears near the fermi energy, which can be tuned by varying the percentage of hydtogen atoms. Therefore functionalized graphene is more useful for applications in nanoelectronics. It is also observed that formation energy increases linearly as the percentage of hydrogen is increased. This inciates that functionalized graphene is more stable and it may be used for hydrogen storage.

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