

Effects of atoms and molecules adsorption on electronic and magnetic properties of s-triazine with embedded Fe atom: DFT investigations

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Abstract

In this paper we employ first-principles calculations to study the mechanical, geometrical, electronic and magnetic properties of Fe atom embedded s-triazine ($Fe@C_6N_6$) system under the influence of external environment. Our result show that the binding energy of $Fe@C_6N_6$ can be modulated by an applied tensile deformation and perpendicular electric field. The non-magnetic semiconducting property of pure s-triazine sheet (C_6N_6) is found to changed upon embeddement of Fe atom in the porous site of the sheet.

1. Introduction

Today, there have been an intense search for the suitable substrates to be used for transition metal (TM) atoms encapsulation [1-3]. The central point in the encapsulation is to ensure that the substrate remains inert and strongly binds to the TM atoms. Moreover, the appropriate substrate is expected to preserve its intrinsic properties and that of bound TM atoms. Two-dimensional (2D) carbon-based and related surfaces with compacted hexagonal rings have been the most frequent choice for trapping TM atoms [4-7]. This is due to their wide surface area. Numerous works have so far been done to investigate the stable geometries and electronic properties of TM atoms adsorption on graphene and boron nitride sheets [7-9]. However, their reports have shown that the adatoms tight weekly on these 2D surfaces as a result of low adsorption energies. Additionally, the large surface free energy of the TM atoms would make them aggregate easily to form cluster on these surfaces. However, forming a regular defect sites experimentally may not be possible due to influence of external environment. Thus, more research efforts have been made to synthesis 2D materials with inherently defined porous sites [10].

2. Results and Discussions

We used the expressions in Eqs. (1) and (2) to compute the mechanical properties, such as in-plane stiffness (Young modulus) and poisson ratio.

$$\text{In-plane stiffness} \quad Y = m_{11} (1 - v^2) \quad (1)$$

$$\text{Poisson's ratio} \quad v = \frac{m_{12}}{m_{11}} \quad (2)$$

The variables m_{11} , m_{12} , (known as elastic constants) can be deduced from Eqs. (3), (4).

$$\text{uni-axial} \quad m_{11} = \frac{1}{A_0} \left(\left(\frac{\partial^2 E}{\partial s^2} \right) \right)_{s=0} \quad (3)$$

$$\text{bi-axial} \quad 2(m_{11} + m_{12}) \frac{1}{A_0} \left(\left(\frac{\partial^2 E}{\partial s^2} \right) \right)_{s=0} \quad (4)$$

where A_0 , E , and s are equilibrium unit-cell area, strain energy and applied deformation. The bulk modulus is determined from the product of equilibrium area and the second gradient of deformation energy with respect to area of the $Fe@C_6N_6$ system, which is written as $G = A \times \left(\left(\frac{\partial^2 E}{\partial A^2} \right) \right)_m$. The variables are defined as follows; A , U and A_m represents the area of the $Fe - C_6N_6$ sheet, the bi-axial deformation energy and the equilibrium area of $Fe@C_6N_6$ respectively. The calculated bulk modulus is less than the value for Mn-CN1 system reported in [1].

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In Table 1 we show the values of binding energy E_b and the structural parameters h and d obtained for different deformations in the range $\pm 2\%$. By applying strain, the height h (difference between the height of Fe and the average height of all atoms in the C_6N_6 sheet) value of the Fe in the relaxed $Fe@C_6N_6$ sheet do not change. Hence, approximately zero h confirms the planar structure of the $Fe@C_6N_6$ sheet.

Acknowledgments

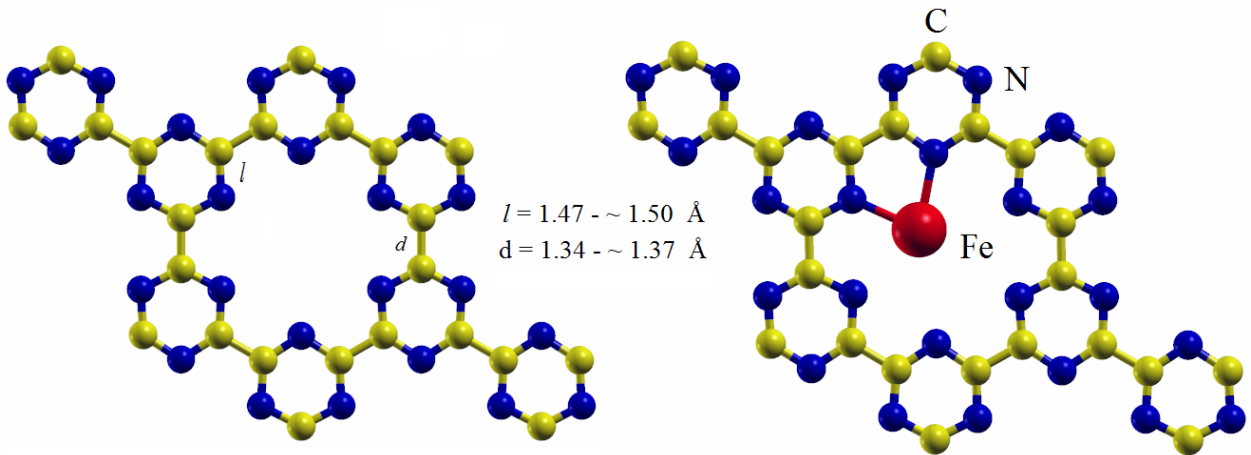
We gladly acknowledge Dr. Chan Huah Yong from the School of Computer Science, USM, for providing us computing resources to carry out part of the calculations done in this paper.

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Table 1. The calculated binding energies E_b , the average bond length between Fe atom and N_{edge} atoms d_{Fe-N} , average bond length connecting the s-triazazine d , and Fe height h (is the difference in the z -coordinate of the Fe atom and the average of the z -coordinate of all the C and N atoms in the C_6N_6 sheet). Charge transfer, magnetic moment per unit cell and per Fe atom, electronic character of the $Fe@C_6N_6$ system are denoted by Q , M_{cell} , M_{Fe} , EC respectively. All the systems are half-metallic.

Strain	E_b (eV)	d_{Fe-N} (Å)	d (Å)	h (Å)	Q (electrons)	M_{Fe} (μ_B)	M_{cell} (μ_B)	EC
0%	4.73	2.06 – 3.40	1.49	-0.01	0.53	3.61	3.74	HM
1%	4.56	2.06 – 3.49	1.51	-0.01	0.54	3.61	3.73	HM
2%	4.05	2.09 – 3.56	1.53	0.00	0.56	3.61	3.71	HM



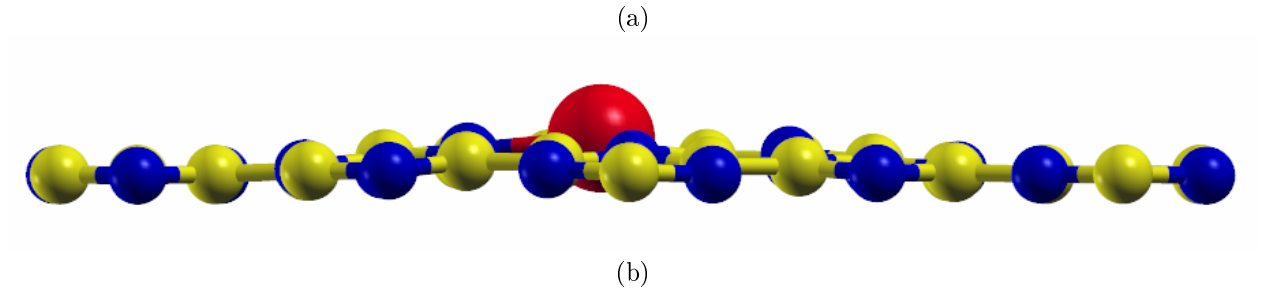


Fig. 1 (a). Relaxed structure of 2×2 C_6N_6 sheet (Left panel) and relaxed structure (Right) of Fe embedded 2×2 C_6N_6 . **(b).** Relaxed side view of 2×2 C_6N_6 sheet with an embedded Fe atom ($Fe@C_6N_6$) under perpendicular electric field strength of 10 V/nm.