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Nitrotyrosine adsorption on defective graphene: A density functional theory study

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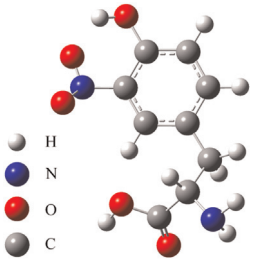
HIGHLIGHTS

- Detection of nitrotyrosine with perfect and defective graphene was studied.
- Structural defects are commonly present in graphene.
- Defects strongly affect the chemical reactivity and electronic properties of graphene.
- Graphene sheets with Stone–Wales, single and double vacancies are semiconductors.
- Defective graphene become n-type semiconductors with nitrotyrosine adsorption.

GRAPHICAL ABSTRACT

Detection of nitrotyrosine with perfect and defective graphene has been studied using density functional theory. Our results provide a good sensor to detect nitrotyrosine which is in connection with Parkinson's disease and Alzheimer's disease.



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ABSTRACT

We have applied density functional theory to study adsorption of nitrotyrosine on perfect and defective graphene sheets. The graphene sheets with Stone–Wales (SW) defect, pentagon–nonagon (5-9) single vacancy, and pentagon–octagon–pentagon (5-8-5) double vacancy were considered. The calculations of adsorption energy showed that nitrotyrosine presents a more strong interaction with defective graphene rather than with perfect graphene sheet. The order of interaction strength is: SW > 5-9 > 5-8-5 > perfect graphene. It is found that the electronic properties of perfect and defective graphene are sensitive to the presence of nitrotyrosine. Hence, graphene sheets can be considered as a good sensor for detection of nitrotyrosine molecule which is observed in connection with several human disorders, such as Parkinson's and Alzheimer's disease.

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1. Introduction

Graphene, which is a hexagonal lattice of carbon atoms, has attracted wide attentions due to its remarkable properties [1]. It has shown wide range of applications such as nanoelectronic devices, energy storage, chemical and biological sensors, etc. [2]. The numerous potential applications of graphene are mainly because of its special electronic property. Many experimental and theoretical efforts showed that the electronic properties of graphene are highly sensitive to the environment conditions [3]. Therefore, several sensors based on graphene have been suggested for detection of small gases such NO_2, NH_3, O_2, and H_2O and large molecules including proteins, DNA, formaldehyde, Nitrotyrosine,

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and organic molecules [4–7].

Nitrotyrosine is a post-translational modified amino acid with different properties than tyrosine or any other of the genetically encoded amino acids. It has been observed in connection with several human disorders such as Parkinson's and Alzheimer's disease [8,9]. Thus, detection of nitrotyrosine during biological processes is a crucial step in diagnosis of progressive disease. In recent years, the possibility of using carbon nanotubes, intrinsic and metal-doped graphene as biosensors for nitrotyrosine detection has been studied using density functional theory [6,10]. The results indicate that the electronic properties of these nanomaterilas are so sensitive to the presence of nitrotyrosine. Hence, carbon nanotubes and graphene are proper sensors for detection of nitrotyrosine during biological processes.

Structural defects which are commonly present in atomic structure of graphene and carbon nanotubes during its growth play a key role in the chemistry and physics of graphene and deteriorate the performance of devices based on graphene and carbon nanotubes [11–18]. In addition, introduction of defects in the carbon network can be useful in some applications. It is an interesting way to tailor intrinsic properties of graphene and create new functionalization [18,19]. The Stone–Wales (SW) defect, single and double vacancies are the most common defects formed in graphene and carbon nanotubes and alter the properties of these nanomaterilas [15–18,20].

It is well-known that defects associated with dangling bonds increase the reactivity of graphene and allow adsorption of other atoms on it [15]. It is also showed that reconstructed defects without dangling bonds such as SW defects or reconstructed vacancies locally changed the density of π-electrons and enhance the local reactivity [20,21]. Structural defects have impact on the bond lengths and curvature around defects which leads to a local rehybridization of σ and π orbitals. All defects cause scattering of the electron waves and change the electron trajectory [22,23]. Therefore, defects strongly affect the electronic properties.

As the presence of defects alters the chemical reactivity and the electronic properties of graphene [13–17], fully exploit of graphene sensors is dependent on considering the effect of defects on the electronic properties of graphene. Recent investigations suggest that the defective graphene can be more suitable for detection of molecules. For instance, it is shown that graphene with SW defect is more sensitive than perfect graphene for formaldehyde detection and the presence of defects enhances the stability of adsorption configurations [5]. Intrigued by this work, we have investigated possibility of using perfect and defective graphene sheets for nitrotyrosine detection in the present work.

2. Computational details

The DFT calculations were performed with the OpenMX3.6 package [24]. The exchange and correlation functions were treated within the generalized gradient approximation (GGA) as parameterized by Perdew–Burke–Ernzerhof (PBE) [25]. The cutoff energy was chosen to be 150 Ry. We have considered 51 k-points along each high symmetry lines of the Brillouin zone. Charge transfer was estimated by means of Mulliken population [26].

To model extended graphene sheet, a supercell of graphene with 98 carbon atoms corresponding to 7×7 unit cells was considered (Fig. 1a) and periodic boundary conditions were applied. This was chosen to keep the separate distance between nitrotyrosine molecules (10 Å) large enough to eliminate their interaction in neighboring supercell. The supercells of graphene were placed inside a large simulation box of $17.23 \times 17.23 \times 14$ Å^3. A vacuum width of 14 Å was considered to avoid interaction between graphene sheets in adjacent boxes.

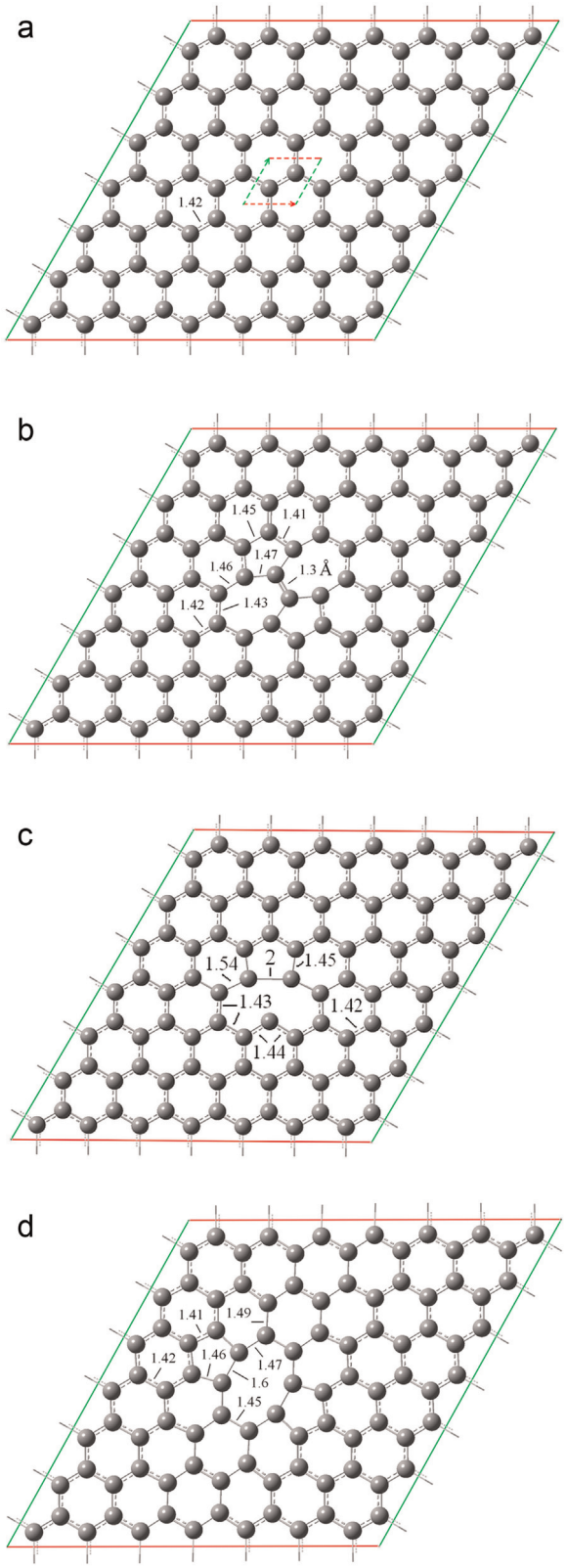

Fig. 1. Illustration of (a) perfect graphene, graphene with (b) SW, (c) 5-9, and (d) 5-8-5 defects.

We have studied graphene with defects such as SW defect, single and double vacancies. As shown in Fig. 1b, SW defect is formed by a simple rotation of one carbon–carbon bond by 90° and consisted of two adjacent pentagon–heptagon pairs (55–77) in which the hexagons share one side. In Fig. 1c and d, snapshots of

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