

# DFT study of hydrogen fluoride and sulfur trioxide interactions on the surface of Pt-decorated graphene

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**Abstract** In this study, we investigate the adsorption properties of hydrogen fluoride (HF) and sulfur trioxide (SO<sub>3</sub>) on the surface of platinum decorated graphene (PtG) using density functional theory. We found one optimized configuration for HF and two ones for SO<sub>3</sub> upon adsorption on the surface of PtG. Our results show significant adsorption on PtG with calculated energy adsorption of  $-73.6$  ( $-54.2$  BSSE) kJ/mol for HF at its only position and  $-172.4$  ( $-144.8$  BSSE) and  $-62.7$  ( $-53.7$  BSSE) kJ/mol for SO<sub>3</sub> at its two positions; P1 and P2, respectively), whereas there is weak physisorption of these analytes on pristine graphene (PG). Results of charge analyses revealed interesting net charge transfer; while the direction of charge is from HF to PtG, reverse direction is found for SO<sub>3</sub> for its two configurations. To deeply understand the concept of adsorption properties, we used orbital analyses including density of states for interaction of mentioned analytes on the surface of PtG.

**Keywords** Pt-decorated graphene · Hydrogen fluoride · Sulfur trioxide · Gas sensor

## Introduction

Graphene has connected carbons in the array of two-dimensional sp<sup>2</sup>. It has excellent properties such as high surface-to-volume fraction [1]. Due to its marvelous electronic structure, it has been used for numerous times as gas

sensor for different analytes [2, 3]. All graphene-made electronic devices benefit from its exceptional charge transferring and its high steadiness. Along with carbon nanotubes [4, 5], there are many experimental and theoretical studies focused on graphene for sensing materials [6–8]. Some research works on graphene as gas sensor were listed and discussed by Mao et al. [9]. They disputed on the opportunities of utilizing these materials for gas sensor purpose.

The properties of graphene could be improved particularly by modification of its surface by doping and decoration of different hetero atoms [10–13]. In our recent study, we have reported the potential of N-doped graphene towards its interaction with boron [14], and SO<sub>x</sub> [15] and CO [16]. We documented that this modified surface is able to increase the adsorption properties of these compounds. Moreover, our group reported different applications of Al and B-doped graphene sheets [17–24]. It has been proved in these papers that metal doping by Al or B increases the adsorbent potential of graphene for practical application.

Besides doping process, metal decoration is another way to intensify the adsorption property of graphene. Upon decoration, single atoms could be placed on high surface area carbons. It will induce the addition of several re-bonding per metal atom with releasing significant energy, which consequently more steadiness of single atom decorated structure in comparison with bulk atoms decorated structure [25]. There are diverse experimental techniques for single atom decoration on nanostructures. As an example, Wang et al. [26] showed that a two-step process is a well-ordered technique to stabilize single atoms on graphene. Diverse metals including Pt, Co, and In, have been successfully incorporated in graphene in the single-atom form. As an example, Baby et al. [27] built an amperometric glucose biosensor by decoration of Pt and

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Au nano-particles on graphene. Based on their research, decorated particles could be able to immobilize glucose oxidase by physical adsorption followed by an enhancement in the performance of biosensor. Moreover, our group searched on the adsorption of NO molecule on the surface of Pt-decorated graphene [28]. We found very high adsorption on this modified surface while there was weak adsorption in the case of using pristine graphene. In parallel we used Pt-decorated graphene as an ideal adsorbent for C<sub>2</sub>H<sub>2</sub> and C<sub>2</sub>H<sub>4</sub> molecules [29], MeOH and EtOH [30], and SO<sub>2</sub> and O<sub>3</sub> [31].

Hydrogen fluoride (HF) is a colorless gas and main industrial source of fluorine, frequently as an aqueous solution named hydrofluoric acid. It is the forerunner for different significant compounds such as polymers (for example Teflon). HF is extensively utilized in the petrochemical industry as a part of super acids. The adsorption of HF on the surface of pristine graphene has been deeply investigated by Sun et al. [32]. They used various configurations for adsorption of HF using DFT and found that at its most energetically favorable site, the amount of adsorption energy is very weak (physisorption).

On the other hand, sulfur trioxide (SO<sub>3</sub>) in the gaseous form is a vital pollutant, which is the primary agent in acid rain. It has been produced on an industrial scale as a precursor to sulfuric acid. Adsorption of SO<sub>3</sub> on pristine graphene has been investigated previously by our group [15]. We found there is very weak adsorption of SO<sub>3</sub> on pristine graphene.

In this study, we select PtG sheet to have more investigation since its potential as adsorbent is well proven. Here we aim to establish the potential of PtG as a new adsorbent for HF and SO<sub>3</sub> molecules by using first-principles simulation. The gas molecules HF and SO<sub>3</sub> are of pollution for industrial as well as environmental applications. They are very poisonous gases and so there is much need for their removal at industrial situations. To the best of our knowledge, there is no reported study on the adsorption properties of HF and SO<sub>3</sub> molecules on the surface of PtG. The inspiration of this study is to attain basic insights to the impact of adsorbed HF and SO<sub>3</sub> molecules on the electronic structure of PtG.

## Computational method

All relaxation for PG and PtG sheets in the present and absence of HF and SO<sub>3</sub> molecules were done using B3LYP density functional with split basis set (for all atoms excluding Pt the basis set was 6-31G (d,p), for Pt atom the basis set was lan12dz) as implemented in Gaussian 09 suite of program [33]. To save the time, initial optimizations were carried by using 3-21G(d)/lan12dz basis set (for all

possible configurations) to distinguish the most stable configurations. Then, among all relaxed structures achieved by this initial functional/basis set, those having highest stability (judging from their calculated adsorption energy) were selected as input files to do next optimization at stronger basis set/functional (6-31G(d,p)/B3LYP) to achieve more precise values of parameters (adsorption energy, equilibrium distance, charge transfer,...).

The 6-31G(d,p) basis set is good for general calculations, besides the B3LYP density functional has been known appropriate for nano-structure studies [28–31].

All calculations including charge analysis, density of states (DOS), the energy of lowest unoccupied molecular orbital (LUMO), the energy of highest occupied molecular orbital (HOMO), and the HOMO–LUMO energy gap ( $E_g$ ) have been done using above-mentioned level of theory.

The values of adsorption energy ( $E_{\text{ads}}$ ) upon adsorption of analyte on PtG were specified using Eq. (1):

$$E_{\text{ads}}(\text{PtG}) = E_{\text{PtG-A}} - (E_{\text{PtG}} + E_{\text{A}}) \quad (1)$$

where the  $E_{\text{PtG-A}}$  corresponds to the adsorbed system of PtG,  $E_{\text{PtG}}$  corresponds to the isolated PtG and  $E_{\text{A}}$  corresponds to the isolated analyte (HF or SO<sub>3</sub>), respectively. For all adsorbed systems, calculated adsorption energies were modified based on the Eq. (2).

$$E_{\text{ads,CP}} = E_{\text{ads}} - E_{\text{BSSE}} \quad (2)$$

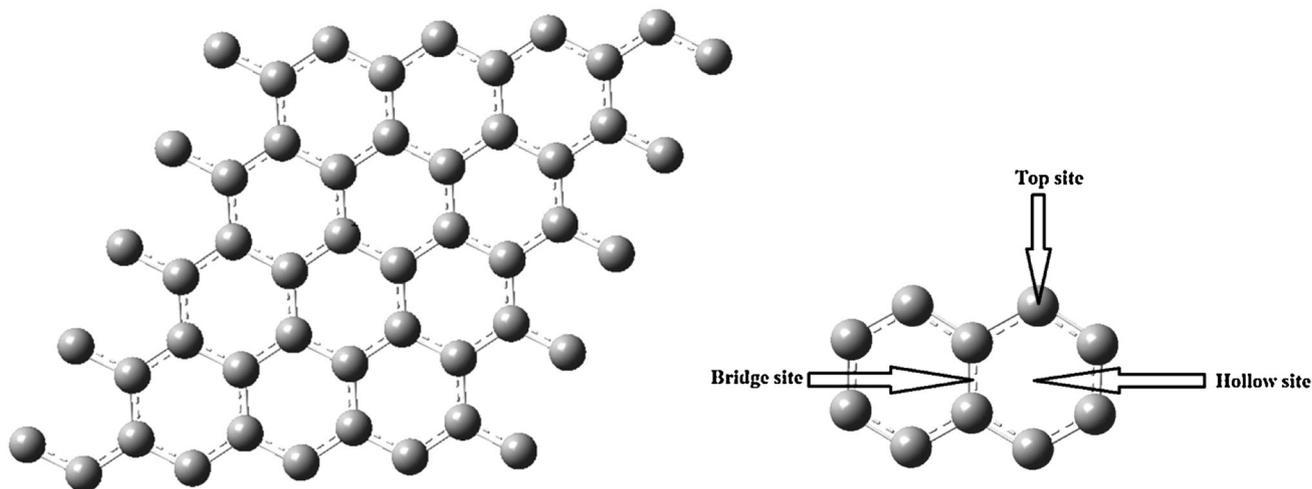
which  $E_{\text{ads,CP}}$  is counterpoise corrected adsorption energy of related complexes and  $E_{\text{BSSE}}$  is basis set superposition errors energy.

## Result and discussions

A supercell of 4 × 4 graphene (12.30 × 12.30 × 16 Å) (left side of Fig. 1) has been used as surface of interaction. There is no interaction between graphene sheets of neighboring supercells since the z axis (16 Å) of this supercell is big enough.

As can be seen in the right side of Fig. 1, there are three potential sites for Pt decoration on graphene: the bridge site (considering the middle of a C–C bond), the top site (directly above a C atom) and the hollow site (at the middle of a hexagon). As we reported in our recent publications [28–31], the bridge site of graphene is the most energetically favorable position for the decoration of Pt compared to the two other ones. Therefore, we placed the Pt atom on this site and let this initial configuration to be optimized at the above-mentioned basis set/functional to make PtG.

As mentioned in the section of introduction, the adsorption properties of both HF and SO<sub>3</sub> on the surface of pristine graphene were investigated before [15, 32] and their relaxed structure were well discussed. For both

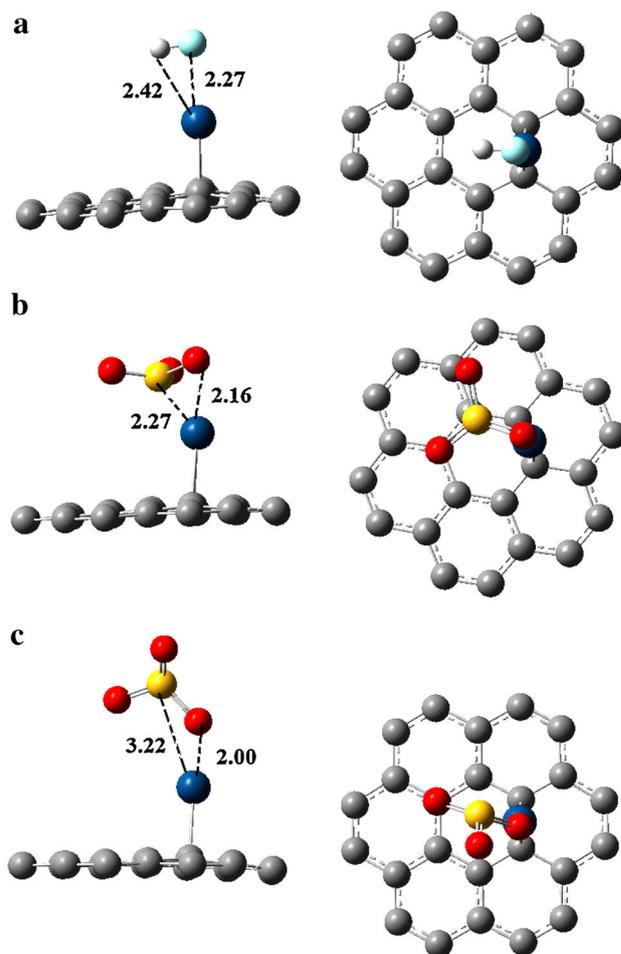


**Fig. 1** A supercell of graphene (*left*) and three possible adsorption sites for decoration of Pt (*right*)

analytes, pristine graphene revealed very low adsorption ( $-7.1$  kJ/mol for HF and  $-9.1$  kJ/mol for  $\text{SO}_3$ , respectively). For this reason, we disregarded to repeat the study of adsorption of these analytes on pristine graphene.

To find the most stable configurations of HF and  $\text{SO}_3$  on Pt-decorated graphene, first we made all possible configurations as input files. For HF, it was placed on top of Pt atom so that the H-F axis in one state has parallel configuration and in other states has perpendicular configurations (one, from the H-side and another, from the F-side) than the surface. Moreover, we placed  $\text{SO}_3$  on top of Pt from the O-side (perpendicular to the surface) and the S-side (parallel to the surface). All these initial configurations were subjected to relaxation at minimum basis set of 3-21G(d) (lanl2dz for Pt) using DFT to primary finding of relaxed structures. We found that all three input structures for HF turn to only one position upon optimization, whereas there are two relaxed structures for output of  $\text{SO}_3$ -including systems. Additionally, we used these initial optimized structures (one for HF and two for  $\text{SO}_3$ ) as input files for next optimization at the stronger basis set of 6-31G(d,p)/(B3LYP, lanl2dz for Pt) to get more precise structure properties. Figure 2 represents the relaxed structures of these adsorbed systems.

Relaxation of HF on PtG accomplishes with releasing  $-73.6$  kJ/mol with closest equilibrium distance of  $2.27$  Å (see Fig. 2). These values are considerable compared to those reported for HF adsorption on pristine graphene (the adsorption energy of  $-7.1$  kJ/mol and adsorption distance of  $3.66$  Å) [32]. Moreover, fully optimization of  $\text{SO}_3$  on PtG corresponds to releasing energies of  $-172.4$  and  $-62.7$  kJ/mol for position 1 and 2, respectively (P1 and P2). The adsorption value of  $\text{SO}_3$  on PtG in both configuration are much higher compared to that reported on pristine graphene ( $-9.1$  kJ/mol) [15]. The closest



**Fig. 2** Side views (*left*) and top views (*right*) of some parts of relaxed structure of adsorbed HF (a) and  $\text{SO}_3$  [P1 (b) and P2 (c)] on PtG

adsorption distances are achieved  $2.16$  and  $2.00$  Å for P1 and P2, respectively, which are completely shorter compared to its adsorption on pristine graphene ( $3.25$  Å) [15].

Despite P1 represents much higher adsorption energy compared to P2, however, the closest adsorption distance of the later is relatively lower than that of P1. This is because in P1, all atoms of  $\text{SO}_3$  involve in formation of bond with Pt, while in P2, only one atom (O) interacts with Pt.

We can conclude that interactions of HF and  $\text{SO}_3$  (in P1 and P2) on PtG could be categorized in chemisorption region. These extensive higher values of HF and  $\text{SO}_3$  adsorption on PtG than their adsorption on PG is a result of high interaction between Pt...F and Pt...O upon their interaction on the earlier surface.

Then, we investigate on the net charge transfer for adsorption of HF and  $\text{SO}_3$  (P1 and P2) on the surface of PtG using natural bond orbital (NBO). The data are listed in Table 1. The net charge transfer for adsorption of HF and  $\text{SO}_3$  were calculated +0.171, -0.337 (P1), and -0.364 (P2) e, respectively. Reverse direction of charge transfer for HF compared to  $\text{SO}_3$  points to the ability of PtG to act

as n-type and p-type semiconductors at the same time. This can be confirmed by considering the local charge of Pt upon adsorption of these analytes (-0.101 e for HF, +0.236 e for  $\text{SO}_3$  (P1), and +0.258 e for  $\text{SO}_3$  (P2), as can be seen in Table 1).

These results accentuate that the adsorption of HF and  $\text{SO}_3$  on PtG significantly change its electronic property.

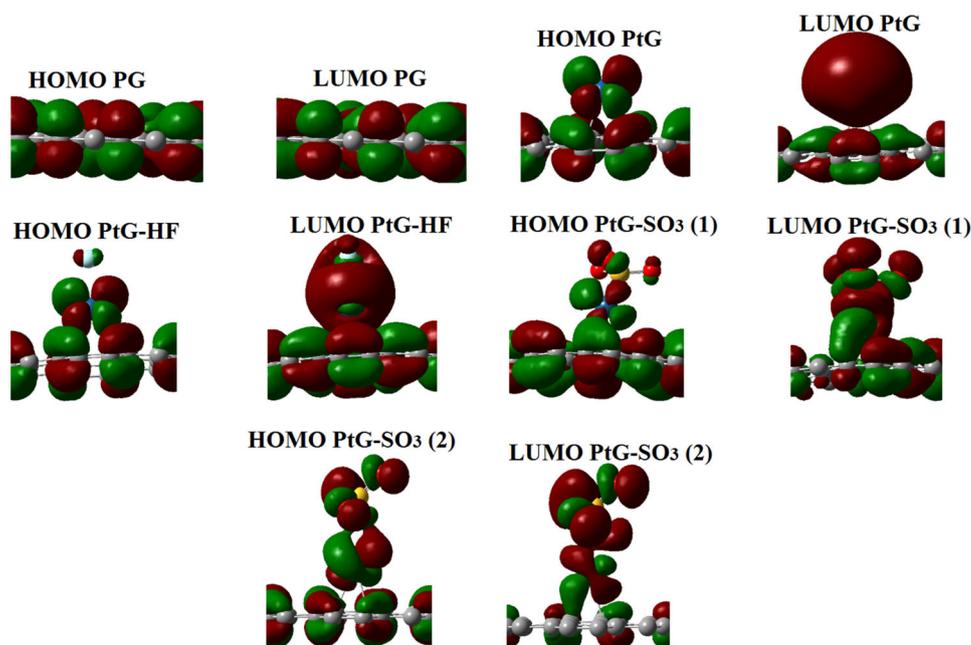
To examine the change in the electronic structure of graphene resulted by decoration of Pt, the HOMO and LUMO distributions of pristine and Pt-decorated graphene sheets are depicted in Fig. 3. It can be seen in Fig. 3, that the HOMO of PG is mostly restricted on the C-C bonds whereas the LUMO is situated on the conflicting site. After Pt is decorated on graphene, major parts of both HOMO and LUMO relocate on Pt atom which result more reactivity of PtG compared to PG. Additionally, the result of NBO analysis showed that the C-atoms neighboring Pt attract charges owing to their high electron affinity and then result a reduce (+0.132 e) in the electron density of Pt.

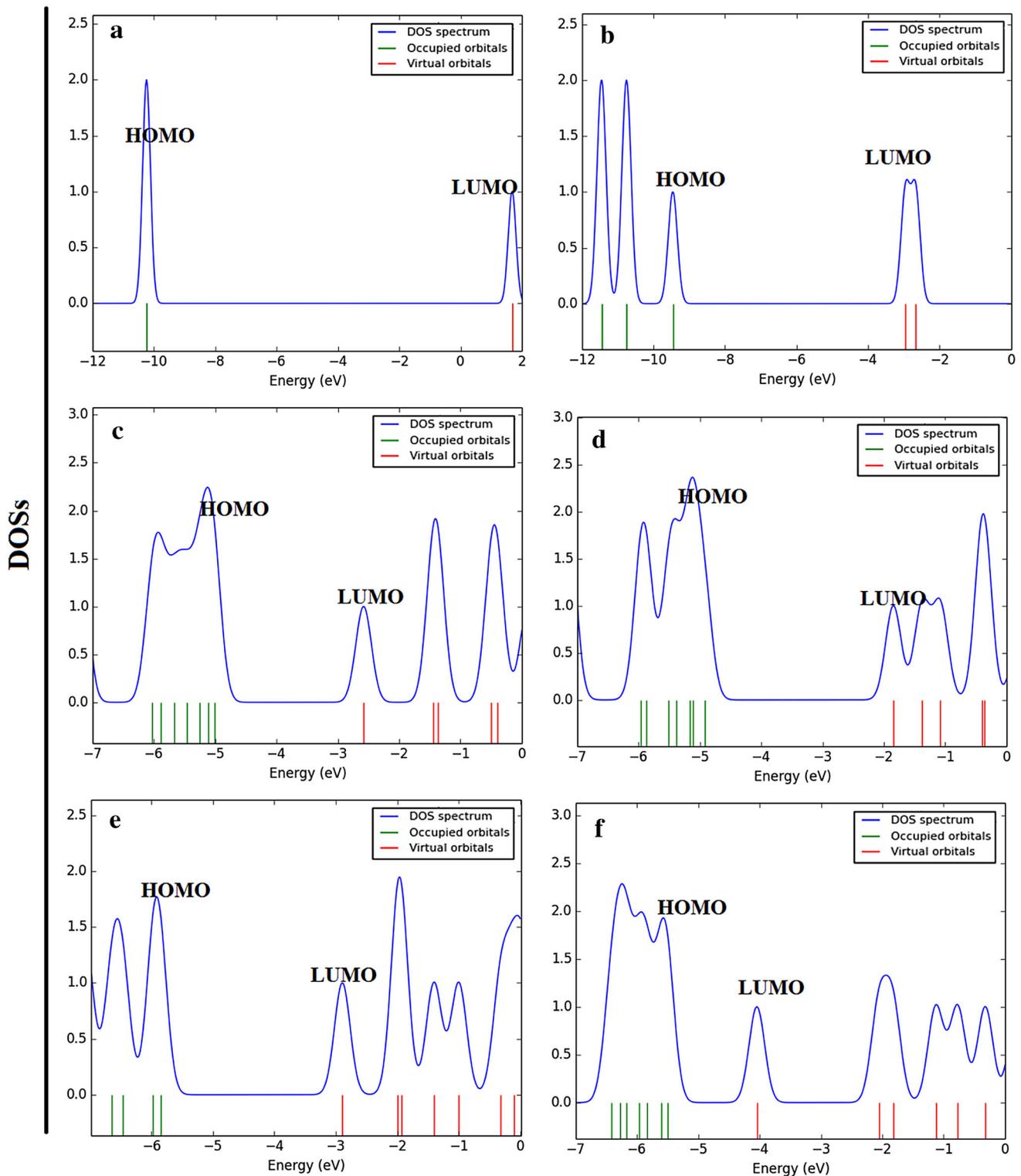
**Table 1** Adsorption energy ( $E_{\text{ads}}$ ) and orbital characteristic:  $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$ , energy of Fermi level ( $E_{\text{FL}}$ ), HOMO-LUMO energy gap ( $E_{\text{g}}$ ), the nearest equilibrium distance ( $d_{\text{e}}$ ) for all systems

System	$E_{\text{HOMO}}$ (eV)	$E_{\text{FL}}$ (eV)	$E_{\text{LUMO}}$ (eV)	$E_{\text{g}}$ (eV)	$Q_{\text{NBO}}$ (e) of adsorbate	$Q_{\text{NBO}}$ (e) of Pt	$d_{\text{e}}$ (Å)	$E_{\text{ads}}$ (kJ/mole)
HF	-10.24		1.68	11.92	-	-	-	-
$\text{SO}_3$	-9.46		-2.96	6.50	-	-	-	-
Isolated PtG	-5.00	-3.79	-2.58	2.42	-	+0.132	-	-
PtG-HF	-4.92	-3.38	-1.84	3.08	+0.171	-0.101	2.27	-73.6 (54.2) <sup>a</sup>
PtG- $\text{SO}_3$ (1)	-5.85	-4.37	-2.89	2.96	-0.337	+0.236	2.16	-172.4 (144.8) <sup>a</sup>
PtG- $\text{SO}_3$ (2)	-5.49	-4.76	-4.04	1.45	-0.364	+0.258	2.00	-62.7 (53.7) <sup>a</sup>

<sup>a</sup> Counterpoise corrected energy

**Fig. 3** HOMO and LUMO distributions of different systems





**Fig. 4** DOSs for free HF (a), free  $\text{SO}_3$  (b), free PtG (c), PtG-HF complex (d), PtG- $\text{SO}_3$  (position 1) (e), and PtG- $\text{SO}_3$  (position 2) (f)

The HOMO and LUMO of adsorbed system for complexed PtG are portrayed in Fig. 3 and the data are listed in Table 1. By comparing the HOMO–LUMO distributions of free PtG with those of adsorbed ones, it can be found that

the distribution of both HOMO and LUMO are effected by adsorbate. These effects are more pronounced in the case of  $\text{SO}_3$  rather than HF as can be expected by their difference in the calculated values of adsorption energy. By

considering the data of Table 1, we can say that upon adsorption of HF, increase in the energies of HOMO and LUMO of system from  $-5.00$  and  $-2.58$  eV to  $-4.92$  and  $-1.84$  eV will happen, respectively. This increase associates with transfer of charge from HF to PtG (p-type semiconductor). On the other hand, for  $\text{SO}_3$  adsorption, the energies of HOMO and LUMO of system decrease to  $-5.85$  and  $-2.89$  eV for P1 and  $-5.49$  and  $-4.04$  eV from their initial values (listed in Table 1). These changes accomplishes with transfer of charge from PtG to  $\text{SO}_3$  (n-type semiconductor).

To deep understanding of the electronic property of PtG upon adsorption of HF and  $\text{SO}_3$ , the DOSs for all systems in free (Fig. 4a, b) and complexed forms were depicted close to the Fermi level (see Fig. 4). Comparing the DOSs of free PtG to that of PtG-HF complex (Fig. 4c, d) we can find significant changes in the location of HOMO and LUMO, in which the  $E_g$  ( $E_{\text{HOMO}} - E_{\text{LUMO}}$ ) of system increase from 2.42 to 3.08 eV. This increase in the  $E_g$  corresponds to increase in the stability of system upon adsorption [34–36].

In the other hand, by comparing the DOSs of free PtG (Fig. 4c) with PtG- $\text{SO}_3$  (Fig. 4c, e, f) important change confirmation of hybridization between  $\text{SO}_3$  and PtG (in both positions) could be find upon adsorption which introduce this modified surface as excellent adsorbent for  $\text{SO}_3$ .

## Conclusion

In this study, we search the adsorption of HF and  $\text{SO}_3$  molecules on the surfaces of PtG. First, we calculated the energy of any relaxed system followed by calculation of orbital descriptions, DOSs and NBO analyses. It was found that the interaction of HF and  $\text{SO}_3$  molecules on PtG changes its electronic structure. The reason for our investigation on PtG was based on knowing this matter of fact that pristine graphene has very weak interaction with these molecules. Decoration of graphene by Pt considerably enhances the potential of graphene to be interacted. The NBO charge analysis reveals reverse direction of charge transfer for  $\text{SO}_3$  compared to HF, pointing PtG is n-type and p-type semiconductors at the same time.

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