



Original Research Article

Adsorption of TNT on the surface of pristine and N-doped carbon nanocone: A theoretical study

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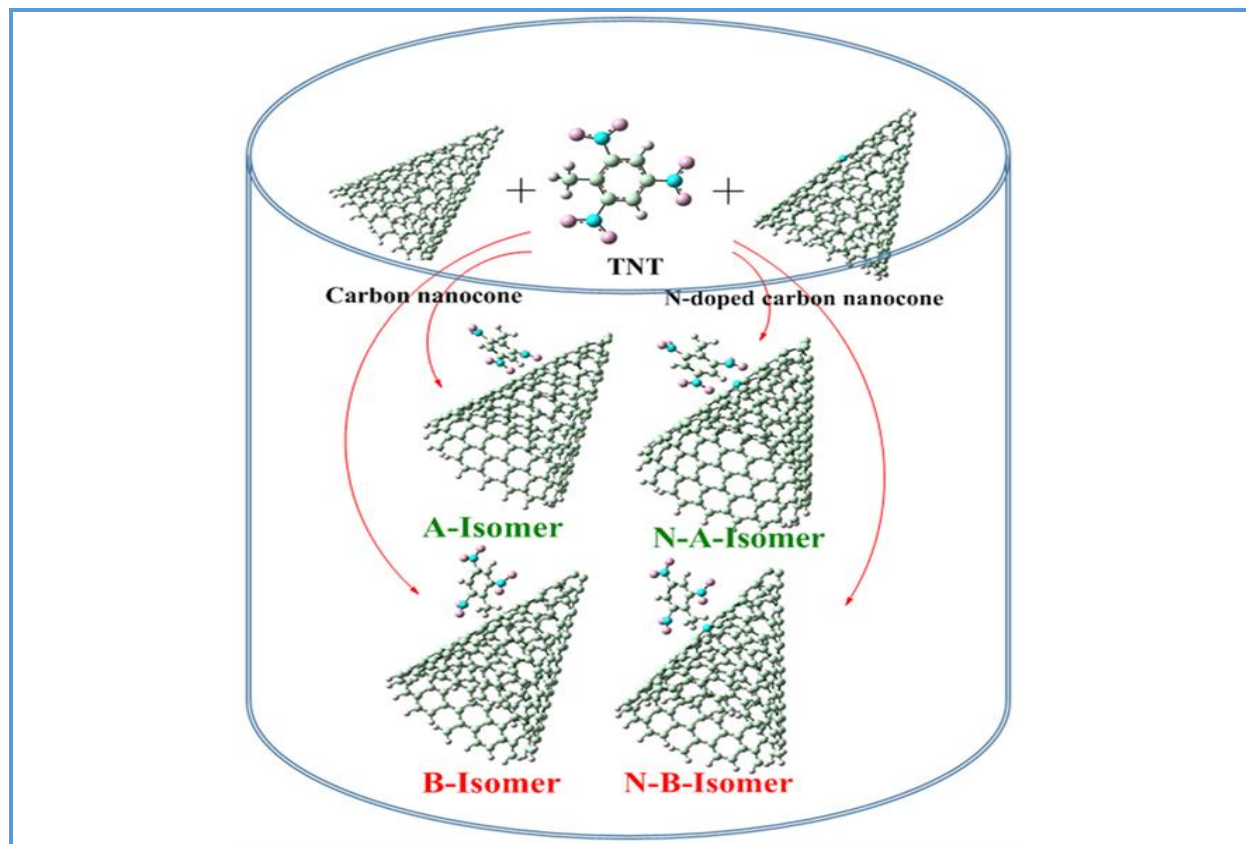
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ABSTRACT

In this research, the performance of the carbon nanocone as an adsorbent and a sensing material for the removal and detection of trinitrotoluene (TNT) was investigated using the density functional theory. The atomic structures of TNT and its complexes with carbon nanocone were optimized geometrically. Infra-red (IR) and frontier molecular orbital computations were employed to evaluate the interaction of TNT with the carbon nanocone. The obtained negative values of adsorption energies, Gibbs free energy changes, adsorption enthalpy variations and great values of thermodynamic equilibrium constants revealed that the interaction of the TNT with carbon nanocone was exothermic, spontaneous and experimentally feasible. The effect of the nitrogen doping and temperature on the adsorption process was also evaluated and the results indicated that TNT interaction with N-doped carbon nanocone was stronger than that of pristine one. In addition, 298 K was the optimum temperature for the adsorption process. The specific heat capacity values revealed that the heat sensitivity was declined tangibly after the TNT adsorption on the surface of carbon nanocone. Besides, the frontier molecular orbital parameters such as bandgap, electrophilicity, maximum transferred charge proved that the carbon nanocone could be utilized as an excellent sensing material for the construction of new electrochemical sensors for TNT determination. Some structural and energetic features were also discussed in details.

Graphical Abstract



Introduction

TNT which its IUPAC name and chemical structure are presented in [Figure 1a](#), is a toxic, carcinogenic and mutagenic explosive. This nitroaromatic environmental contaminant has been extensively used as a powerful energetic compound in the production of war bombs and as a chemical intermediate for the synthesis of the photographic compounds and dyes [1–4]. Therefore, pollution of air, soil, water and foods with TNT is a serious problem in the areas that are adjacent to the ammunition plants and some industrial towns [5–7]. According to the former reports, TNT can cause crucial health problems including liver damage, aplastic anemia, renal irritation, peripheral neuritis, skin hemorrhages, arrhythmia and various types of cancer for the people who are exposed to it [8–

11]. In this respect, determination and removal of TNT are very crucial. In addition, in recent decades, terroristic activities have extended in many countries [12–14]. Therefore, quantitation of commonly used explosives like TNT that plays a key role in finding a clue for hidden terroristic activities and improving the security.

Several methods have been reported for determination of TNT including chemiluminescence, fluorimetry, high-performance liquid chromatography (HPLC), gas chromatography coupled with mass spectrometry (GC-MS), surface-enhanced Raman spectroscopy and ion mobility spectrometry (IMS) [15–18]. Although, the referred techniques have high sensitivity and low detection limits, their instrumentations are too intricate and expensive. Moreover, the

mentioned methods were found to be time-consuming and needed high-experienced operators for performing the sophisticated sample preparation steps before the main analysis. In addition, large amounts of toxic organic solvents are used in the analysis procedures of these methods [19–21].

Fortunately, electrochemical and thermal sensors are good alternatives for the cited techniques. These types of sensors are simple, portable, economical, rapid, highly selective and applicable for colored and opaque specimens [22]. However, the most crucial step in the development of new sensors is exploiting a novel recognition element that has a selective and strong interaction with the desired analyte [23–25].

On the other hand, carbon nanocone which its structure is presented in Figure 1b, was discovered by Ge and Sattler in 1994 [26–28]. Carbon nanocone is considered as an intermediate between graphene and carbon nanotube that can be synthesized by cutting 1-5 sectors of angle 60° from a graphene sheet connecting the originated edges by the cut, with 1-5 pentagons at the aspects. This carbon-based nanostructure has a high surface/volume ratio, prominent mechanical stability and high electrocatalytic activity. These properties make carbon nanocone an ideal candidate for several applications such as removing the contaminants and sensors [29–37]. In this regard, the performance of carbon nanocone for the removal and detection of TNT and the effects of this nanostructure on the energetic features of TNT was investigated using the density functional theory for the first time, in this research.

Computational details

At first, the structures of TNT and carbon nanocone were designed by Gauss View 3.1 and Nanotube modeller 1.3.0.3 software

respectively [31]. Their structures were optimized geometrically. Then IR and frontier molecular orbital computations were performed on them. All of the computations were implemented in the Gaussian 09 software by density functional theory method and in the B3LYP/6-31G (d) level of theory [11–13].

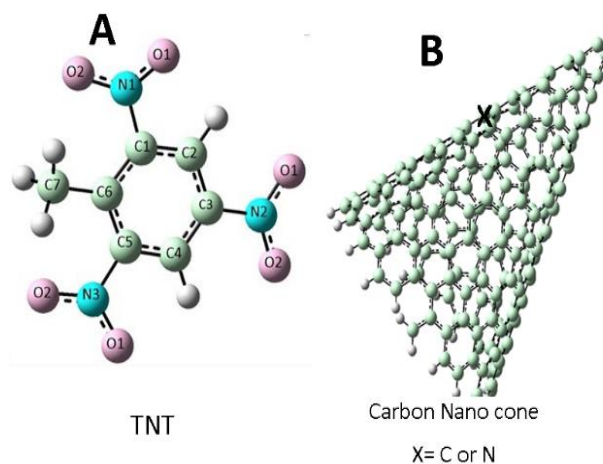
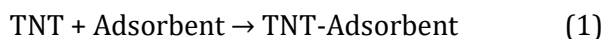


Figure 1. a) The structures of TNT, b) pristine and nitrogen-doped carbon nanocone

This basis set was selected because in the previous researches, the obtained theory results from this level of theory were in a great agreement with the real experimental data [14]. All of the computations were done in the aqueous phase and in the temperature range of 298.15–398.15 K at 10° intervals. The evaluated process can be shown schematically by the following equation:



Equations 2–5 were utilized to calculate the values of adsorption energy (E_{ad}), and important thermodynamic parameters of the investigated process such as adsorption enthalpy changes (ΔH_{ad}), Gibbs free energy variations (ΔG_{ad}) and thermodynamic equilibrium constants (K_{th}) respectively [15–17].

$$E_{ad} = (E_{(TNT-Adsorbent)} - (E_{(TNT)} + E_{(Adsorbent)})) \quad (2)$$

$$\Delta H_{ad} = (H_{(TNT-Adsorbent)} - (H_{(TNT)} + H_{(Adsorbent)})) \quad (3)$$

$$\Delta G_{ad} = (G_{(TNT-Adsorbent)} - (G_{(TNT)} + G_{(Adsorbent)})) \quad (4)$$

$$K_{th} = \exp(-\Delta G_{ad} / RT) \quad (5)$$

Where, E is the total electronic energy of each structure, H stands for the sum of the thermal correction of enthalpy and total energy of the evaluated materials, G represents the sum of the thermal correction of Gibbs free energy and total energy for each of the studied structures, R is the ideal gas constants and T denotes the temperature.

Frontier molecular orbital parameters including bandgap (HLG), chemical hardness

(η), chemical potential (μ), electrophilicity (ω) and the maximum transferred charge (ΔN_{max}) were calculated using the Equations 6-10 [18-20].

$$HLG = E_{LUMO} - E_{HOMO} \quad (6)$$

$$\eta = (E_{LUMO} - E_{HOMO})/2 \quad (7)$$

$$\mu = (E_{LUMO} + E_{HOMO})/2 \quad (8)$$

$$\omega = \mu^2 / 2\eta \quad (9)$$

$$\Delta N_{max} = -\mu / \eta \quad (10)$$

E_{LUMO} and E_{HOMO} in Equations 6 to 8, represent the energy of the lowest unoccupied molecular orbital and the energy of the highest occupied molecular orbital consecutively.

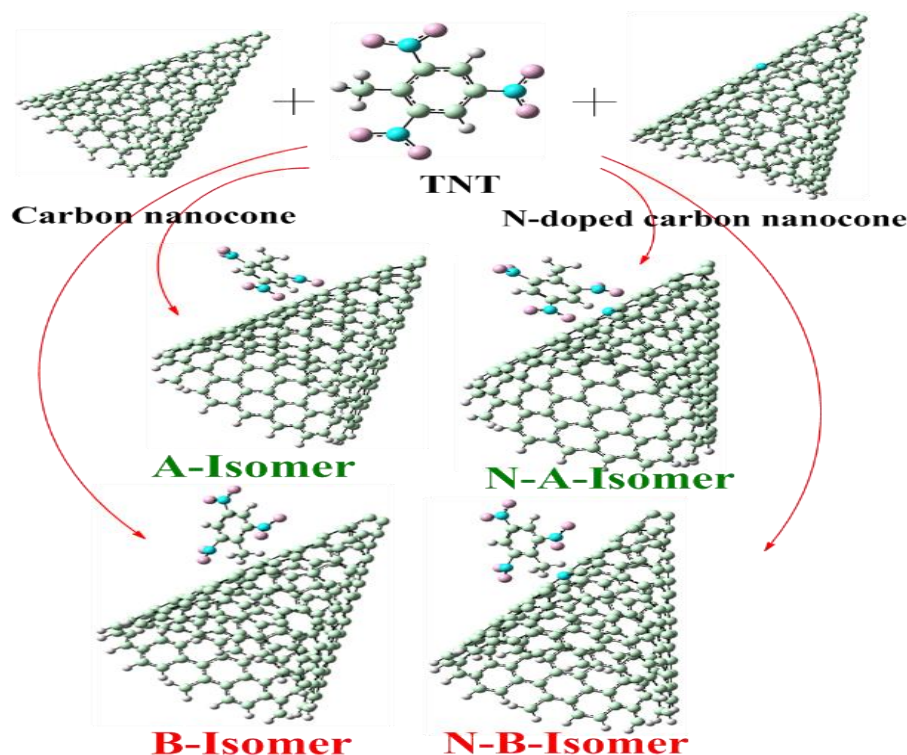


Figure 2. The Optimized Structures of TNT and its Complexes with pristine and nitrogen-doped carbon nanocone

Results and Discussion

As seen in Figure 2, TNT interaction with carbon nanocone was evaluated at two different situations to find the most stable configuration. Then, the carbon nanocone was doped by nitrogen in both configurations. Nitrogen was selected as the dopant atom as nitrogen-doped carbon nanostructures have been synthesized experimentally and N-doping usually leads to a tangible improvement in the features of these nanomaterials. For better understanding, an abbreviated name was considered for each configuration and the naming method is explained in the following:

The A-Isomer and N-A-Isomer names were considered for the derivatives that were created from the interaction of the second carbon atom of TNT benzene ring with the pristine and nitrogen-doped carbon nanocone respectively. In these conformers, the benzene ring of TNT was inserted near the surface of the adsorbent in parallel form but after geometrical optimizations, TNT was oriented toward the adsorbents from the sixth carbon atom of the TNT benzene ring. It seems that a chemical bond was formed between the second carbon atom and the adsorbents. The B-Isomer and N-B-Isomer names were assigned to the derivatives

Structural features

produced from the interaction of TNT methyl group with the pristine and N-doped carbon nanocone consecutively.

The values of total electronic energy, adsorption energy, the lowest frequency, bond lengths and zero-point energy for TNT and its complexes with the adsorbents are presented in Table 1. As the provided data reveal clearly, the adsorption energy values for all of the configurations are negative which indicating that the adsorption process is experimentally possible. Due to the fact that the adsorption energy values were lower than 200 KJ/mol, it seems that TNT adsorption is a chemisorption process [11]. In other words, a chemical bond was formed between the adsorbate and the adsorbent in this case. The low C-C and C-N bond lengths are another proof for TNT chemisorption on the surface of pristine and N-doped carbon nanocone [13]. The next important point that can be realized from the reported adsorption energies is that after doping carbon nanocone with nitrogen the interaction of TNT with the adsorbents improved significantly because of the remarkable decline in the adsorption energy values after nitrogen doping [12].

Table 1. The values of total electronic energy, adsorption energy, the lowest frequency, zero-point energy and bond lengths for TNT and its complexes with pristine and nitrogen-doped carbon nanocone

+	TNT	A-Isomer	B -Isomer	N-A-Isomer	N-B--Isomer
Total energy (a.u)	-868.580	-1615.672	-1615.617	-1631.514	-1631.454
Adsorption energy (KJ/mol)	---	-701.720	-556.551	-1017.862	-861.589
Lowest frequency (cm ⁻¹)	45.029	24.116	7.557	15.306	6.553
C ₁ -N ₁ (Å)	1.512	1.615	1.616	1.672	1.675
C ₃ -N ₂ (Å)	1.512	1.613	1.614	1.691	1.693
C ₅ -N ₃ (Å)	1.506	1.612	1.615	1.682	1.685
N ₁ -O ₁ (Å)	1.278	1.368	1.364	4.186	1.474
N ₁ -O ₂ (Å)	1.278	1.361	1.369	1.632	1.482
N ₂ -O ₁ (Å)	1.278	1.369	1.356	1.477	1.478
N ₂ -O ₂ (Å)	1.278	1.364	1.369	1.479	1.478

N ₃ -O ₁ (Å)	1.278	1.359	1.378	1.477	1.478
N ₃ -O ₂ (Å)	1.278	1.381	1.368	1.470	1.478
C ₇ -C (Å)	---	1.474	---	---	---
C ₂ -C (Å)	---	---	1.434	---	---
C ₇ -N (Å)	---	---	---	1.363	---
C ₂ -N (Å)	---	---	---	---	1.395
Zero point energy (KJ/mol)	394.351	628.892	623.014	681.923	679.741

The C-NO₂ and N-O bond lengths in nitroaromatic explosives is a good criterion for evaluating the energetic properties of this type of materials. As can be seen in Table 1, when TNT adsorbs on the surface of pristine and nitrogen-doped carbon nanocone, the C-NO₂ and N-O bond lengths increased. This phenomenon means TNT complexes with carbon nanocone can participate in combustion and explosion processes more conveniently in

comparison to the pure TNT [28–30]. In fact, the explosion power of TNT has improved after its interaction with carbon nanocone and this improvement in the case of N-doped complexes is more sharply because the mentioned bond lengths have increased in nitrogen-doped complexes more than the pristine ones. Therefore, carbon nanocone can be used for synthesizing new energetic composites with better explosive features [25].

Thermodynamic parameters of adsorption process

The values of adsorption enthalpy changes (ΔH_{ad}) were calculated using Equation 3 and the obtained results are depicted in Table 2. As seen in Table 2, the interaction of TNT with carbon nanocone is exothermic in both of the evaluated configurations. The next important point that can be realized from Table 2, is that TNT has a stronger interaction with nitrogen-doped carbon nanocone in comparison with that of the pristine one. This is due to the fact that after doping the nano-adsorbent with nitrogen the values of ΔH_{ad} have declined dramatically [21]. The effect of temperature on the adsorption process of the TNT was also assessed. As observed, by increasing the temperature the ΔH_{ad} values have become more positive indicating that the TNT adsorption has become

less exothermic at high temperatures. Due to the fact that the TNT interaction with carbon nanocone is so exothermic and a considerable amount of heat was produced in this procedure, carbon nanocone can be used for the development of new thermal sensors for detection of this explosive [22]. In thermal sensors, the desired analyte participate in an interaction with a sensitive recognition element and if the interaction is highly exothermic, the released heat will change the temperature of the environment. Then, the temperature variations can be measured using a sensitive thermistor [23]. Therefore, the produced signal (temperature alterations) have a direct relationship with the concentration of the analyte.

Table 2. The values of adsorption enthalpy changes (ΔH_{ad}) in the temperature range of 298.15-398.15 k at 10° intervals

Temperature (K)	ΔH_{ad} (KJ/mol)			
	A-Isomer	B-Isomer	N-A-Isomer	N-B-Isomer
298.15	-776.046	-635.536	-1010.096	-1322.368

308.15	-776.043	-631.225	-1008.119	-1316.612
318.15	-776.002	-626.984	-1006.248	-1310.891
328.15	-775.945	-622.811	-1004.481	-1305.219
338.15	-775.891	-618.736	-1002.817	-1299.578
348.15	-775.821	-614.736	-1001.234	-1293.979
358.15	-775.755	-610.820	-999.739	-1288.397
368.15	-775.687	-606.968	-998.301	-1282.820
378.15	-775.641	-603.204	-996.935	-1277.299
388.15	-775.614	-599.529	-995.664	-1271.825
398.15	-775.567	-595.917	-994.459	-1266.432

The Gibbs free energy change (ΔG_{ad}), was calculated using Equation 4, and the results are depicted in Table 3. As can be seen, the TNT adsorption on the surface of carbon nanocone was spontaneous at both of the configurations. As it is clear, by doping carbon nanocone with nitrogen the TNT interaction with the proposed interaction has become more spontaneous as the values of (ΔG_{ad}) have become more negative. Therefore, it seems that the nitrogen-doped carbon nanocone is a better adsorbent for the removal of this toxic nitroaromatic compound. The influence of temperature on this parameter was also investigated. As can be seen, the optimum temperature for the TNT adsorption process is 298.15 K, as the lowest (ΔG_{ad}) values have been achieved in this temperature [26].

The thermodynamic equilibrium constants (K_{th}) of the adsorption process were also calculated using Equation 5 and the obtained data are tabulated in Table 4. TNT interaction

with carbon nanocone was found to be one-sided, irreversible and non-equilibrium due to the positive obtained values [14-16]. The main advantage of K_{th} is that it depicts the role of temperature more evidently compared to that of the other thermodynamic parameters. As can be observed, the values of K_{th} reduced substantially as the temperature enhanced. Therefore, TNT interaction with carbon nanocone was found to be stronger at the ambient temperature. This phenomenon is not out of expecting because energetic compounds such as TNT are not stable at high temperature and it will participate in the combustion and explosion reactions [27]. The TNT interaction with nitrogen-doped carbon nanocone was more irreversible than its interaction with pristine carbon nanocone because after replacing the carbon atoms of the adsorbent with nitrogen the values of K_{th} was increased tangibly.

Table 3. The values of Gibbs free energy changes (ΔG_{ad}) in the temperature range of 298.15-398.15 k at 10° intervals

Temperature (K)	ΔG_{ad} (KJ/mol)			
	A-Isomer	B-Isomer	N-A-Isomer	N-B-Isomer
298.15	-705.866	-568.276	-933.107	-1154.055
308.15	-703.543	-566.008	-930.291	-1150.042
318.15	-701.147	-563.720	-927.519	-1145.982
328.15	-698.659	-561.367	-924.740	-1141.822
338.15	-696.150	-558.946	-922.001	-1137.613
348.15	-693.626	-556.504	-919.232	-1133.396
358.15	-691.071	-554.005	-916.419	-1129.072
368.15	-688.478	-551.497	-913.589	-1124.731

378.15	-685.931	-549.002	-910.751	-1120.348
388.15	-683.523	-546.552	-907.846	-1115.856
398.15	-681.037	-544.079	-904.939	-1111.391

Table 4. The values of thermodynamic equilibrium constants (K_{th}) in the temperature range of 298.15-398.15 k at 10° intervals

Temperature (K)	K_{th}			
	A-Isomer	B-Isomer	N-A-Isomer	N-B-Isomer
298.15	4.669E+123	3.657E+99	3.037E+163	1.559E+202
308.15	1.829E+119	8.866E+95	5.010E+157	8.938E+194
318.15	1.319E+115	3.599E+92	1.940E+152	1.435E+188
328.15	1.644E+111	2.297E+89	1.602E+147	5.766E+181
338.15	3.462E+107	2.211E+86	2.681E+142	5.438E+175
348.15	1.180E+104	3.147E+83	8.352E+137	1.135E+170
358.15	6.214E+100	6.341E+80	4.577E+133	4.745E+164
368.15	4.872E+97	1.784E+78	4.251E+129	3.865E+159
378.15	5.655E+94	6.880E+75	6.434E+125	5.776E+154
388.15	9.713E+91	3.581E+73	1.501E+122	1.479E+150
398.15	2.243E+89	2.411E+71	5.325E+118	6.493E+145

The applicability of many explosives has become limited due to their high sensitivity to heat and thermal shock. In this regard synthesis of new composites with a lower heat sensitivity is of great importance. The specific heat capacity (C_v) is defined as a certain amount of heat that is needed for increasing the temperature of a substance to one centigrade degree [16]. Therefore, a compound with a high value of C_v should gain more energy to increase its temperature. In this regard, C_v has a direct relationship with heat sensitivity of explosives. For this reason, this parameter was also

computed for TNT and its derivatives with pristine and nitrogen-doped carbon nanocone and the results are presented in Table 5. As the provided data showed clearly, the C_v value of TNT increased sharply after its adsorption on the surface of pristine and N-doped carbon nanocone. Thus, the heat sensitivity of TNT has abated after its adsorption on the carbon nanocone and this nanostructure is a prominent material for synthesizing novel energetic composites of TNT with lower heat sensitivity [13].

Table 5. The values of specific heat capacity (C_v) for TNT and its derivatives with pristine and N-doped carbon nanocone in the temperature range of 298.15-398.15 k at 10° intervals

Temperature (K)	C_v (J/mol.K)				
	TNT	A-Isomer	B-Isomer	N-A-Isomer	N-B-Isomer
298.15	198.991	417.154	423.710	400.091	400.091
308.15	203.629	428.343	434.647	410.486	410.486
318.15	208.217	439.363	445.421	420.715	420.715
328.15	212.753	450.209	456.029	430.777	430.777
338.15	217.238	460.880	466.469	440.673	440.673
348.15	221.670	471.370	476.736	450.403	450.403
358.15	226.048	481.677	486.829	459.968	459.968
368.15	230.371	491.798	496.744	469.366	469.366

378.15	234.638	501.730	506.479	478.600	478.600
388.15	238.848	511.472	516.031	487.670	487.670
398.15	242.999	521.021	525.399	496.575	496.575

Frontier molecular orbital analysis

The energy of the highest occupied molecular orbital (HOMO), and the energy of the lowest unoccupied orbital (LUMO) were investigated using the frontier molecular orbital computations. In addition, some structural properties including energy gap (HLG), chemical hardness (h), chemical potential, electrophilicity (ω), maximum transferred charge (ΔN_{\max}) for TNT and its complexes with the evaluated adsorbent were calculated using Equations 6-10 respectively and the results are presented in Table 6. The energy gap is defined as the energy discrepancy between HOMO and LUMO molecular orbitals and has a direct relationship with the conductivity and electrocatalytic activity of compounds [16]. In fact, the molecules with a low energy gap can transfer their electrons from the valence layer to the conduction layer easier than the molecules with a considerable large amount of energy gap. As can be seen, when TNT interacts with the pristine carbon nanocone the HLG experiences a tangible increase [21]. Therefore, the electrical conductance has reduced when TNT adsorbs on the surface of pristine carbon nanocone. However, when TNT adsorbs on the surface of nitrogen-doped carbon nanocone, this parameter has declined remarkably which is a proof for enhancing of electrical conductivity in the interaction process. Hence, the variations in the electrical conductivity in both cases could be used as a signal for the detection of TNT. In this regard, pristine and N-doped carbon nanocone are applicable for construction of novel electrochemical sensors for determination of TNT [24].

The chemical hardness of the studied compounds was also evaluated because of its

relevance to the reactivity of the molecules. The soft molecules which have a low amount of h can change their electron density more comfortably than the hard molecules with high values of h . Thus, electron transmissions that are essential for the implementation of chemical reactions can be done in the soft substances conveniently [11]. As it is obvious, after TNT adsorbed on the surface of the pristine carbon nanocone this parameter has increased significantly however, in the case of nitrogen-doped carbon nanocone, the value of chemical hardness was reduced. Therefore, it can be concluded that the TNT complexes with nitrogen-doped carbon nanocone have higher reactivity than that of the pure TNT. On the other hand, the reactivity of TNT complexes with the pristine adsorbent was lower than the pure TNT [13]. Electrophilicity and maximum transferred charge are good standards for estimating the affinity of molecules toward electrons. As the provided data in the table shows clearly, all of the TNT complexes with pristine and N-doped carbon nanocone have lower amounts of electrophilicity and maximum transferred charge than the pure TNT. Therefore, the tendency of TNT for electron absorbing has decreased after its interaction with the adsorbents. The next point that can be understood from the table is that TNT plays the role of an electron acceptor or a lewis acid but pristine and N-doped carbon nanocone plays the role of an electron donor or a lewis base in the adsorption process [20]. In other words, an electron transfer process can be done in the adsorption process. In this regard, carbon nanocone can be used as an ideal sensing material for detection of TNT. Dipole moment has a clear relationship with the solubility of the

compounds. As can be observed, this parameter has enhanced after TNT adsorption on the surface of the adsorbents. In other words, TNT

complexes with pristine and nitrogen-doped carbon nanocone have better solubility in polar solvents in comparison to the pure TNT [21].

Table 6. The values of E_H and E_L , HLG, Chemical hardness (h), Chemical potential (μ), electrophilicity index (ω), maximum transferred charge (ΔN_{max}) and dipole moment for TNT and its complexes with carbon nanocone

	E_H (eV)	E_L (eV)	HLG(eV)	η (eV)	μ (eV)	ω (eV)	ΔN_{max} (eV)	Dipole moment (deby)
TNT	-8.060	3.290	11.350	5.675	-2.385	0.501	0.420	1.110
Carbon nanocone	-6.290	2.870	9.160	4.580	-1.710	0.319	0.373	1.280
A-Isomer	-8.080	5.870	13.950	6.975	-1.105	0.088	0.158	2.070
B-Isomer	-8.440	5.750	14.190	7.095	-1.345	0.127	0.190	4.870
N-doped-carbon nanocone	-7.850	4.650	12.500	6.250	-1.600	0.205	0.256	2.540
N-A-Isomer	-7.370	3.270	10.640	5.320	-2.050	0.395	0.385	5.140
N-B-Isomer	-7.530	3.060	10.590	5.295	-2.235	0.472	0.422	3.980

Conclusions

TNT is a toxic nitroaromatic compound causing serious environmental problems and endangering the health of humans and other living organisms. Therefore, its removal and determination are very significant. In this regard, TNT adsorption on the surface of carbon nanocone was evaluated in this study using the density functional theory. The values of adsorption energies, enthalpy changes, Gibbs free energy variations and thermodynamic equilibrium constant showed TNT interaction with carbon nanocone was found to be exothermic, spontaneous, non-equilibrium and experimentally feasible. The effect of temperature on the thermodynamic parameters was also studied and the findings showed that the TNT adsorption process had the highest yield in the room temperature. The effect of doping carbon nanocone with nitrogen was also investigated and the results indicated that TNT interaction with N-doped carbon nanocone was found to be stronger than that of the pristine nano-adsorbent. The specific heat

capacity values that substantiated the heat sensitivity of TNT declined after its adsorption on the surface of carbon nanocone. The C-N and N-O bond lengths proved that TNT energetic traits improved substantially after its interaction with carbon nanocone. The values of energy gap proved that carbon nanocone is an ideal sensing material for the fabrication of novel electrochemical sensors for TNT quantitation. Due to the fact that the theoretical results showed the capability of the pristine and N-doped carbon nanocone as a prominent adsorbent and sensing for removal and detection of TNT, it is recommended to the experts of these fields to investigate these subjects experimentally.

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Disclosure Statement

No potential conflict of interest was reported by the authors.

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