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Optoelectronical Properties of a Metalloid-Doped $B_{12}N_{12}$ Nano-Cage

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Abstract: The opteoelectronical properties of $B_{12}N_{12}$ nano-cage was investigated in the present of some metals by density functional theory (DFT). After the adsorption of a toxic molecule with all complexes, the electronic properties in $B_{11}GeN_{12}$ nano-cage were significantly increased. The UV-Vis adsorption and Infrared spectroscopy of cyanogen chloride over the $B_{11}GeN_{12}$ have been performed by the time-dependent density functional theory (TD-DFT). The increasing of λ_{max} values from the pristine $B_{12}N_{12}$ to $B_{11}GeN_{12}$, reveals that $B_{11}GeN_{12}$ nano-cages can be a suitable structure as optic sensor for this gas detection. Overall, Because of the crystalline defect, Symmetry disruption and the changes in the degree of polarization, the semiconductor property affects these nano-cage systems. Finally, the changes of energy of gap (E_g) with a significant charge transfer from this gas to Ge-doped nano-cage, which lead to changes of conductance of it and render this kind of system sufficient for gas detection.

Keywords: $B_{12}N_{12}$ nano-cage, Opteoelectronical Properties, IR and UV-Vis Spectroscopies, TD-DFT Method.

1. INTRODUCTION

$B_{12}N_{12}$ fullerene is made up of four-hexagons and six squares and belongs to the elements of groups III and V in the periodic table is also an interesting subject of the most researchers [1-3]. For the first time, BN fullerenes were synthesized by Stéphan et al. [4]. Then, $B_{12}N_{12}$ fullerene was synthesized by an arc-melting method from YB_6 powder in N_2/Ar mixture gas [5]. Recently, several studies have been reported on BN fullerene materials because of their excellent properties including; low dielectric constant, wide-band gap, high-temperature stability, oxidation resistance, and large thermal conductivity [6-8].

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In contrast with the other fullerenes, $B_{12}N_{12}$ is one of the best known stable classes of fullerenes with the network of boron-nitrogen bonds, which is energetically remarkable [9]. The presence of single isolated atom impurities and dopants adsorbed on the inner and outer surfaces of BN fullerenes can effectively enhanced the electronic properties of these nanomaterial's [10]. Metal-doped BN cages were also studied experimentally [11] and theoretically [12-13]. A better conception of the metal-fullerene interaction will have potential influences upon applications including catalysis, sensors, fabrication of core-sheath nanostructures and nanoelectronics [14]. Tazikeh have studied the optical and electronical properties of aluminum nitride nano-cages sensitive to some gases such as; Cl_2 [15] and NH_3 molecules [16]. Also, they have investigated the interaction of pure and carbon atom substituted boron nitride fullerenes with ifosfamide drug [17]. Soltani and co-workers have demonstrated, gas chemical sensor based on boron nitride nanocages [18]. They found that the electronic properties of $B_{12}N_{12}$ under an electric field have significant changes toward adsorption of N_2O and leads to the conductivity changes of $B_{12}N_{12}$. The interaction of CO molecule toward pure and doped $B_{11}XN_{12}$ (X = Mg, Ge, Ga) nano-cages was investigated, too [19]. Before, we indicated the Al and Ga-doped BNNTs interacted with cyanogen chloride molecule which is good candidates for the detection of this gas molecule [20]. Baei et al. have studied the cyanogen chloride molecule adsorption toward the perfect, Al-, and B-doped C_{60} fullerenes using DFT calculations. They found that the electronic property of the B-doped C_{60} fullerene was dramatically altered on the cyanogen chloride molecule adsorption [21]. Recently, the adsorption of cyanogen chloride molecule molecule on different nano-materials including AlNNT, graphene and C_{20} fullerene were reported [22, 23]. In the past years, the studies have been purposed on the pure and metal-doped $B_{12}N_{12}$ nano-cages and their application in drug delivery system and the detection of many toxic gas molecules [24- 27].

The aim of this research was the adsorption study of the cyanogen chloride molecule on the pure and metal-doped (Mg, Al, and Ge) $B_{12}N_{12}$ nano-cages as sensing materials for detection of this toxic gas by using density functional theory (DFT) computations and UV-Vis spectroscopy, too.

2. COMPUTATIONAL METHOD

The geometries and electronic properties of the pure and metal-doped $B_{12}N_{12}$ systems were studied by using PBE method as implemented in Gaussian 09 software package [28]. Moreover, PBE functional which belongs to the generalized gradient approximation functional for exchange-correlation energy has been previously proved to have good dependability in computing molecular binding energies of the gas molecules on boron nitride nanostructures [29-31]. Structural relaxation was performed upon all complexes with a convergence

criterion for the energy of 10^{-5} Ha/atom. Gauss Sum package [32] was used to analyze the density of state (DOS) plots. The binding energy (E_{Bind}) of the cyanogen chloride molecule adsorbed on the $B_{12}N_{12}$ nano-cages was computed by subtracting of the total energy of the nano-cage and cyanogen chloride molecule from the energy of their complexes. Thus, the negative E_{Bind} demonstrates that the calculated system is stable and the positive one corresponding local minimum where the interaction of cyanogen chloride molecule onto the considered $B_{12}N_{12}$ nano-cages is prevented by a barrier. To determine the opteoelectronical properties, the UV-Vis absorption have been accomplished by the time-dependent density functional theory (TD-DFT) calculations at the PBE functional and 6-311++G (d,p) basis set for the most stability of nano-cages.

3. RESULTS AND DISCUSSION

The optimum energy of all systems of cyanogen chloride molecule from on the pure and Mg, Al, Ge-doped $B_{12}N_{12}$ nano-cages were calculated and We have found the most stable state for the cyanogen chloride on $B_{12}N_{12}$ nano-cage with metal-doped belongs to Ge metal. Nagarajan and Chandiramouli have shown the interaction of cyanogen chloride on blue phosphorene nanosheet and arsenene nanoribbon with the adsorption energies of -0.65 and -0.55 eV, respectively [33, 34]. After full relaxation, we have found only one most stable adsorbed state in which the N atom of cyanogen chloride by weak electrostatic bonds is connected to one B atom of the nanocage with small-distance of 1.621 Å. Mulliken population charge analysis (MPA) demonstrates a weak charge transfer about 0.044 |e| from the molecule to $B_{12}N_{12}$ nanocage, which is in agreement with the calculated results by the Rouhani [35]. This can be evaluated by the MEP image of the cyanogen chloride molecule, suggesting that the electrostatic potential on the N atom is greatly more negative than that on the Cl atom and it tends to attack the electron-deficient region of the boron sites [36]. As shown in Table 1, in the process of physisorption, cyanogen chloride molecule is weakly adsorbed on the nano-cage with insignificant changes in geometry. This was in quite an agreement with other results by Baei and Soltani [37-39]. After adsorption process, the length of B–N bond has risen from 1.494 to 1.564 Å and the N–B–N bond angle has reduced from 98.48° to 92.69° in pure $B_{12}N_{12}$, respectively. To alter the reactivity, adsorption behavior and electronic sensitivity of the $B_{12}N_{12}$ nano-cages to the cyanogen chloride molecule, a boron atom is substituted by three metal atoms including Mg, Al and Ge. Recently, many authors have been published on the replacing a B atom by these atoms in the wall of BN nanostructures [40-42]. It has been shown that replacing a boron atom by Al one is significantly more effective than replacing a nitrogen atom [43-45]. Optimized geometries of all these structures, including the cyanogen chloride, pure, and Mg, Al, and Ge-doped $B_{12}N_{12}$ nanocages were

calculated by DFT calculations. The relaxed geometries of the $B_{11}MgN_{12}$, $B_{11}AlN_{12}$, and $B_{11}GeN_{12}$ nano-cages demonstrate that the length of Mg-N, Al-N, and Ge-N bonds are lengthened by about 2.081, 1.847, and 1.946 Å, respectively, while the length of B-N bond is about 1.494 Å. The assessment of aspirin adsorption onto the pure and Al-doped $B_{12}N_{12}$ nano-cages was studied by Vessally et al. [46]. They have shown the distance between N and Al atoms for the $B_{11}AlN_{12}$ is 1.82 Å which is longer than the bond length between B and N in the $B_{12}N_{12}$ system. In a study by Soltani and Javan [12], the length of Ga–N, Ge–N, and Mg–N bonds of the Mg, Al and Ge-doped $B_{12}N_{12}$ nano-cages are computed with values of 1.921, 1.946, and 2.079 Å, respectively. These results are in agreed with present results. Table 1, is shown the cyanogen chloride adsorption on the outer surfaces of $B_{11}MgN_{12}$ and $B_{11}AlN_{12}$ are chemisorption, while the adsorption of this gas on the $B_{11}GeN_{12}$ surface is physisorption. The larger negative of E_{Bind} (-1.38 eV) indicate that the cyanogen chloride from its nitrogen head present strong chemical interaction with the $B_{11}AlN_{12}$ nano-cage compared to $B_{11}MgN_{12}$ and $B_{11}GeN_{12}$, thus the stable adsorbed system are formed. The arrangements of the adsorbed cyanogen chloride molecule on the pure and metal-doped $B_{12}N_{12}$ nano-cages are obtained analogous results on the pure and Al-doped blue phosphorene nano-sheet [33] and the Al-doped boron nitride nanostructures [36]. For the most stable adsorption system, the increment of dipole moment (DM) observed for the $B_{11}AlN_{12}$.

Table I, represent the value of HOMO and LUMO energies (eV) for the cyanogen chloride adsorbed on the pure and Mg, Al, Ge-doped $B_{12}N_{12}$ nano-cages. The more changes in HOMO and LUMO energies appeared on the replacing a B atom by the Al_B atom compared to a form of other doping atoms (Mg_B and Ge_B) in $B_{12}N_{12}$ nano-cage. It was found that addition of Ge_B to boron nitride monolayer leads to higher energies in the valence and conduction band states. Before, Gupta et al. have studied similar computation [47] by using C and Ge doped BN monolayers at the DFT-PBE [48-50]. Upon the interaction of cyanogen chloride with metal-doped nano-cages, the HOMO and LUMO energies have more changes in $B_{11}GeN_{12}$ nano-cage compared to $B_{11}MgN_{12}$ and $B_{11}AlN_{12}$ nano-cages. The most changes of HOMO and LUMO energies is correspond to a reduction in the E_g (energy of gap) of $B_{11}GeN_{12}$- cyanogen chloride complex (2.73 eV) compared to that of the pure $B_{11}GeN_{12}$ system (3.67 eV). According to DOS plots in Al- and Ge-doped B12N12, the most changes in the HOMO and LUMO happened near Fermi level (E_F) which causes reduction in the E_g values. Therefore, $B_{11}Ge\ N_{12}$ has the highest change in the E_g (ΔE_g) with a value of 60.80% in comparison with other states (see Table 1).

Our calculations reveal that the electronic properties of the $B_{11}GeN_{12}$ nano-cage are very sensitive to the cyanogen chloride molecule compared to the $B_{12}N_{12}$ nano-cage.

The UV-Vis absorption spectrum of cyanogen chloride adsorbed over the $B_{11}GeN_{12}$ and $B_{11}GeN_{12}$ complexes with cyanogen chloride have been performed by the time-dependent density functional theory (TD-DFT) calculations at the PBE functional and 6-311++G(d,p) basis set. The calculated maximum absorption wavelengths (λ_{max}), the corresponding oscillator strengths (f_{osc}), and excitation energies (ΔE) of all investigated $B_{11}GeN_{12}$ and $B_{11}GeN_{12}$ complexes with cyanogen chloride gas. The estimated values of λ_{max} and ΔE for the $B_{12}N_{12}$ system is increased from 206 nm with f_{osc} of 0.0012 to 295 nm and 0.0141 after adding of Ge atom to the nano-cage. The estimated minimum absorption wavelengths for the $B_{11}GeN_{12}$ nano-cage are found to be 380 nm (0.0055) and 608 nm (0.0086). Abdolahi *et al.* reported that the absorption spectrum of $B_{12}N_{12}$ fullerene at the wavelengths of 204 and 205 nm by M06-2X functional [25, 27]. In Fig. 3, for A and B states, the maximum peaks decreased to 303 nm (0.0998) and 414 nm (0.0164), respectively. For the states A and B, ΔE values are reduced to 4.08 eV (A) and 2.99 eV (B) compared to the pure $B_{11}GeN_{12}$ nano-cluster (4.20 eV), respectively (Table Ⅱ). The calculation reveals that $B_{11}GeN_{12}$ can be suitable as optic sensor for the cyanogen chloride detection.

4. CONCLUSION

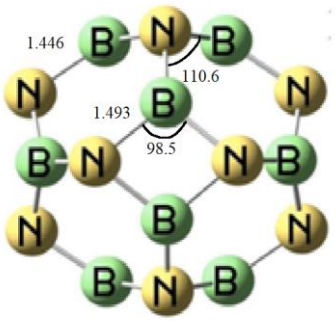
The adsorption behavior of the cyanogen chloride molecule on the pure, Mg-, Al-, and Ge-doped $B_{12}N_{12}$ nano-cages was calculated and reported by using DFT calculations. It was found that, before the interaction of cyanogen chloride molecule from its nitrogen head can be chemically adsorbed over the surface of $B_{11}AlN_{12}$ compared to $B_{12}N_{12}$, $B_{11}MgN_{12}$ and $B_{11}GeN_{12}$ nano-cages. Compared to the pure $B_{12}N_{12}$, the interaction of cyanogen chloride molecule from its nitrogen head with the Al atom from $B_{11}AlN_{12}$ (E_{ads} = -1.38 eV) is strong compared with the $B_{11}MgN_{12}$ (E_{ads} = -1.07 eV). After the interaction of this toxic molecule with $B_{11}GeN_{12}$, their electronic properties are significantly increased. In addition, the changes of E_g with a significant charge transfer from this gas molecule to the $B_{11}GeN_{12}$, which lead to changes of conductance of nano-cage and render this kind of system sufficient for gas detection. The calculation reveals that $B_{11}GeN_{12}$ can be suitable as optic sensor for this gas detection.

TABLE I. The electronic parameters of the pure and metal-doped $B_{12}N_{12}$ nano-cages with the presence and absence of cyanogen chloride.

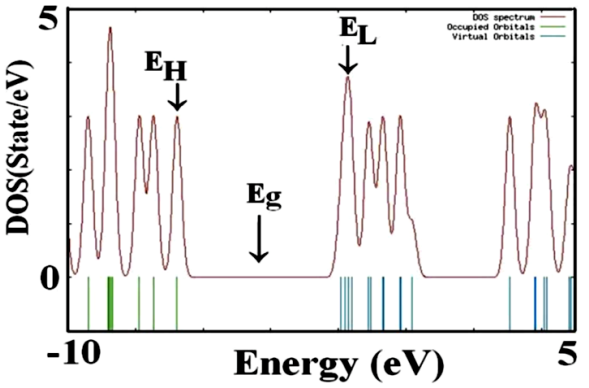
Property	**$B_{12}N_{12}$**	**$B_{12}N_{12}$ + cyanogen chloride**	**$B_{11}MgN_{12}$**	**$B_{11}MgN_{12}$ + cyanogen chloride**	**$B_{11}AlN_{12}$**	**$B_{11}AlN_{12}$ + cyanogen chloride**	**$B_{11}GeN_{12}$**	**$B_{11}GeN_{12}$ + cyanogen chloride**
E_{ad} (eV)	-	-0.45	-	-0.12	-	-0.24	-	-0.22
DM (Debye)	0.0	9.71	5.44	12.44	3.37	10.59	1.78	9.80
E_{HOMO} (eV)	-7.03	-6.14	-6.20	-6.27	-6.63	-5.82	-6.47	-5.65
E_{LUMO} (eV)	-2.04	-3.01	-3.03	-3.03	-3.77	-3.82	-2.80	-2.92
E_g (eV)	4.99	3.13	3.17	3.24	2.86	2.0	3.67	2.73
ΔE_g (%)	-	37.27	36.47	2.16	42.69	43.0	26.45	60.80
E_F (eV)	-4.54	-4.58	-4.62	-4.65	-5.2	-4.82	-4.64	-4.29

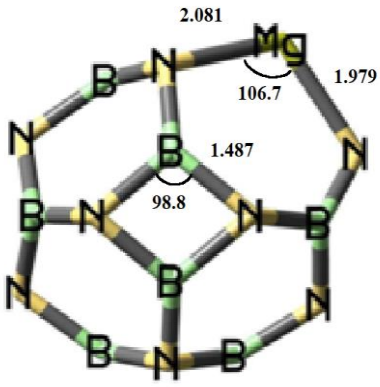
TABLE Ⅱ. The energy changes (ΔE), oscillator strengths (f_{osc}) and absorption wavelength (λ) of the pure and Ge-doped in $B_{12}N_{12}$ nano-cages by UV-Vis spectroscopy.

Property	**$B_{12}N_{12}$**	**$B_{11}GeN_{12}$**	**(I)**	**(Ⅱ)**
λ (nm)	206	295	303	414
f_{osc}	0.0012	0.0141	0.0998	0.0164
ΔE (eV)	-	4.20	4.08	2.99

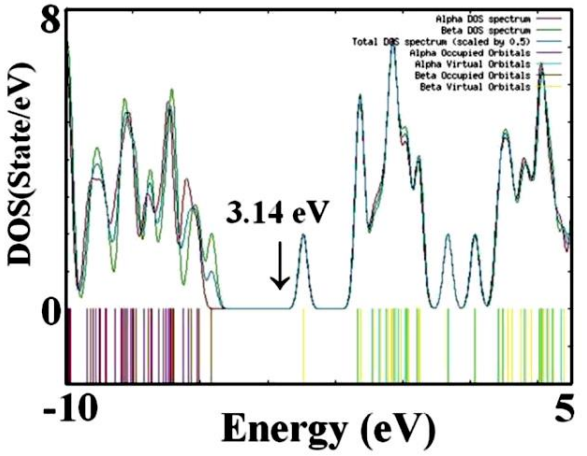


B12N12





B11MgN12



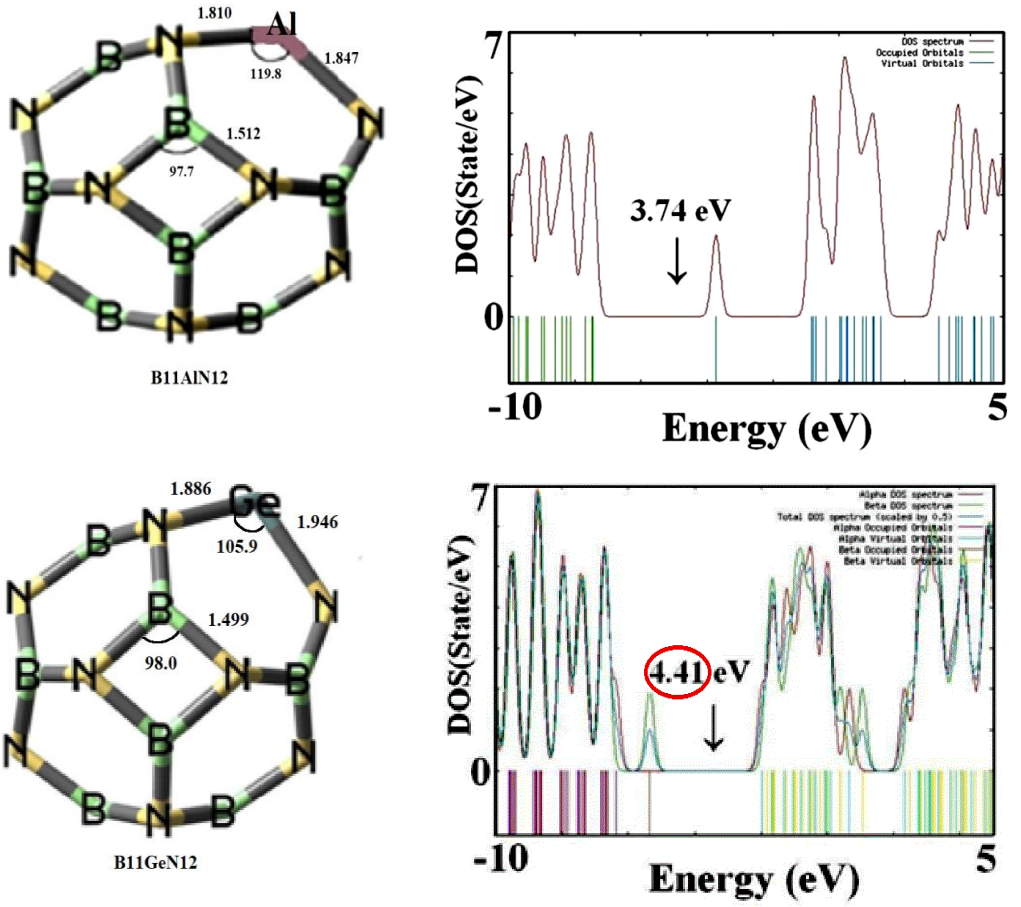


Fig. 1. The geometrical parameters and density of states (DOS) of pure and (semi) metal-doped $B_{12}N_{12}$ nano-cages. All bond distances and angles are in Å and °, respectively.

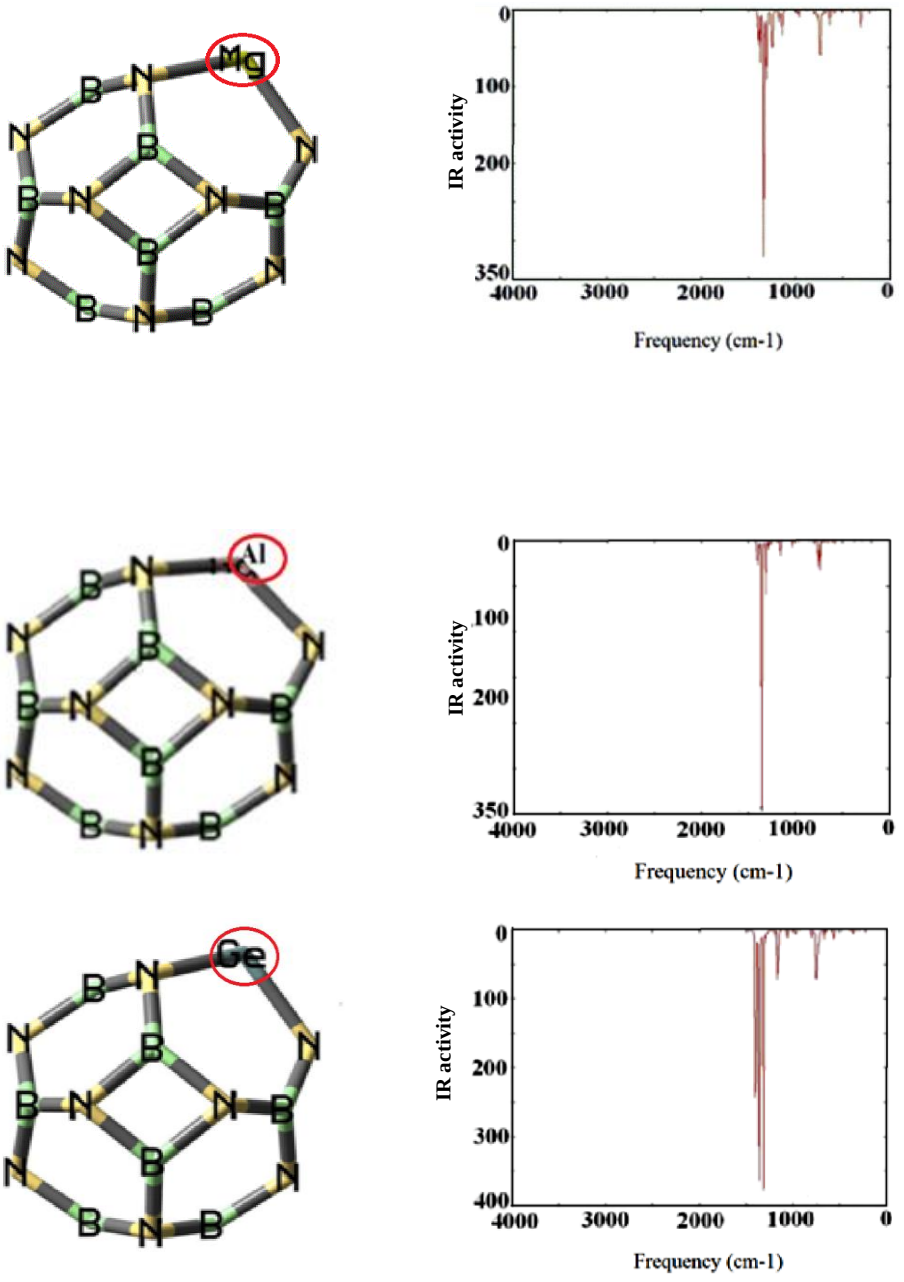
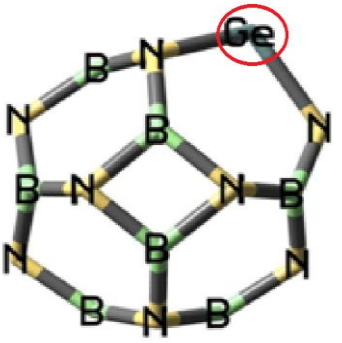
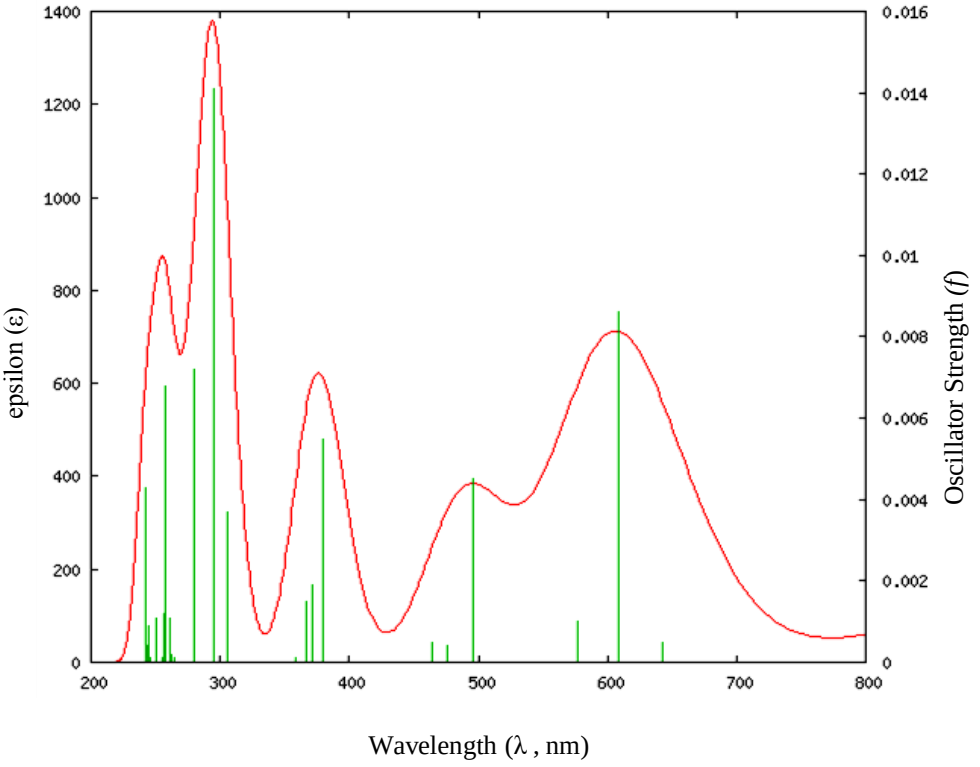


Fig. 2. The theoretical IR spectra of cyanogen chloride gas adsorbed on (semi) metal-doped $B_{12}N_{12}$ fullerene in the compared with other metals.


Ge
B
N


epsilon (ε)
Oscillator Strength (f)
Wavelength (λ , nm)
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200
400
600
800
1000
1200
1400
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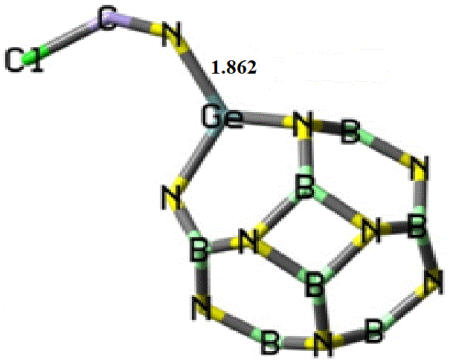
0.004
0.006
0.008
0.01
0.012
0.014
0.016
200
300
400
500
600
700
800


C
N
Cl
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Ge
N
B
N
B
N
B
N
B
N
B
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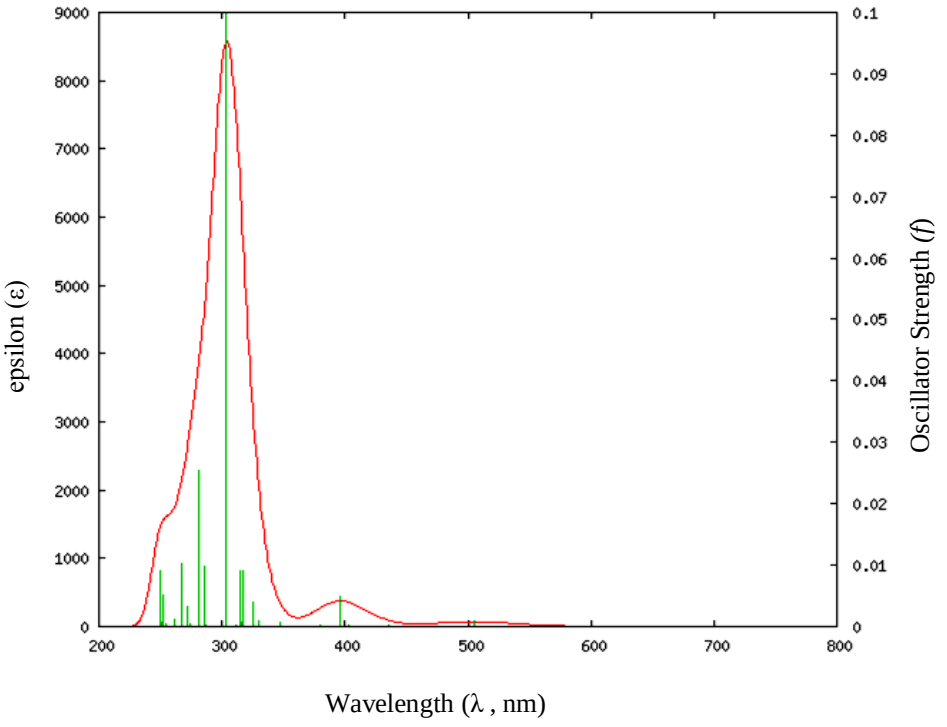
N
B
N
B


epsilon (ε)
Oscillator Strength (f)
Wavelength (λ , nm)
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8000
7000
6000
5000
4000
3000
2000
1000
0
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
200
300
400
500
600
700
800

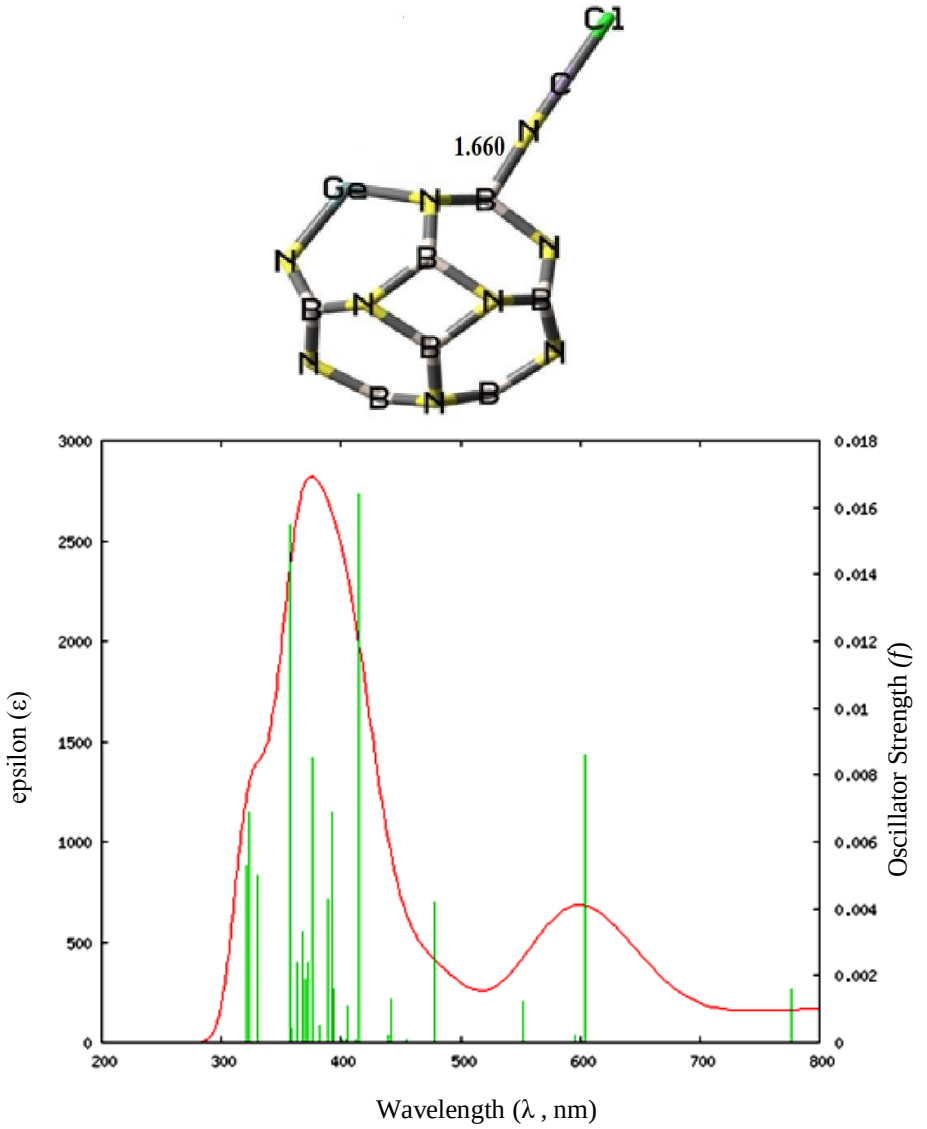

Fig. 3. UV-Vis spectrums for $B_{11}GeN_{12}$ nano-cages in the absence and presence of cyanogen chloride gas, which is determined by a Gaussian functional convolution using by Gauss Sum 2.2.5 software, FWHM = 3000 cm^{-1}. Excitation energy, Oscillator strength (f_{osc}) and absorption wavelength (λ, nm) calculated through 6-311++G (d,p) level.

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